Superconductivity near the Mott transition

T. Senthil (MIT)

Superconductivity, its friends and its enemies, near the Mott transition

T. Senthil (MIT)

Useful other Boulder lectures

Cuprate phenomena + some theory

1. M. Randeria, http://boulderschool.yale.edu/sites/default/files/files/Randeria-Boulder-Lecture1.pdf

2. S. Kivelson, 2014

3. A. Paremakanti, 2014

Quantum spin liquids, quantum criticality.

1. TS, http://boulder.research.yale.edu/Boulder-2008/Lectures/Senthil/Boulder1.pdf

2. Patrick Lee, http://icam-i2cam.org/index.php/research/file/lee1

Plan

Lecture 1

1. Examples of superconductivity and related phenomena near Mott transition

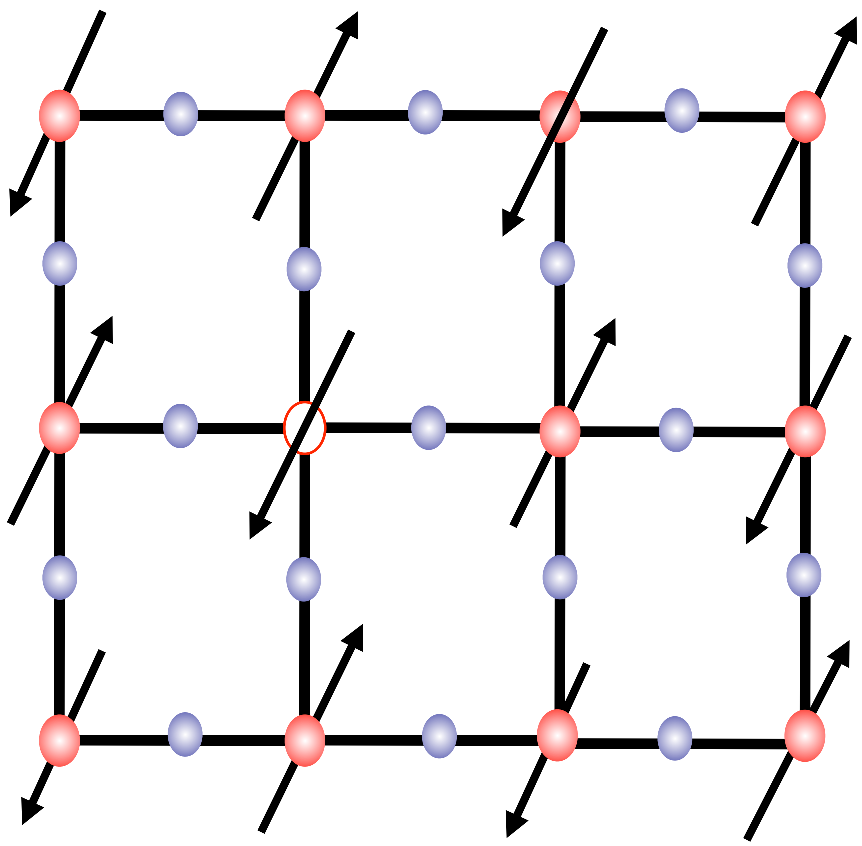
2. Magnetism and Mott insulators

Lecture 2

Metals and superconductors near the Mott transition

-(i) some general questions
-(ii) some theoretical answers.

What is a Mott insulator?



Insulation due to jamming effect of Coulomb repulsion

Coulomb cost of two electrons
occupying same atomic orbital dominant

⇒Electrons can’t move if every possible atomic
orbital site is already occupied by another electron.

Odd number of electrons per unit cell: band theory predicts metal.

Useful theoretical model: the Hubbard model

Electrons on lattice sites i with 1 electron per site on average

$$H = -t \sum_{<ij>} \left(c_i^\dagger c_j + h.c \right) + U \sum_i \frac{n_i(n_i - 1)}{2}$$

Electron hopping

Electron repulsion

$n_i =$ number of electrons at site i.

$t \gg U$: Hopping wins; Fermi liquid metal.

$U \gg t$: Repulsion wins; Mott insulator

Complications in many real Mott insulators

1. Orbital degeneracy: More than one atomic orbital may be available for the electron to occupy at each site.

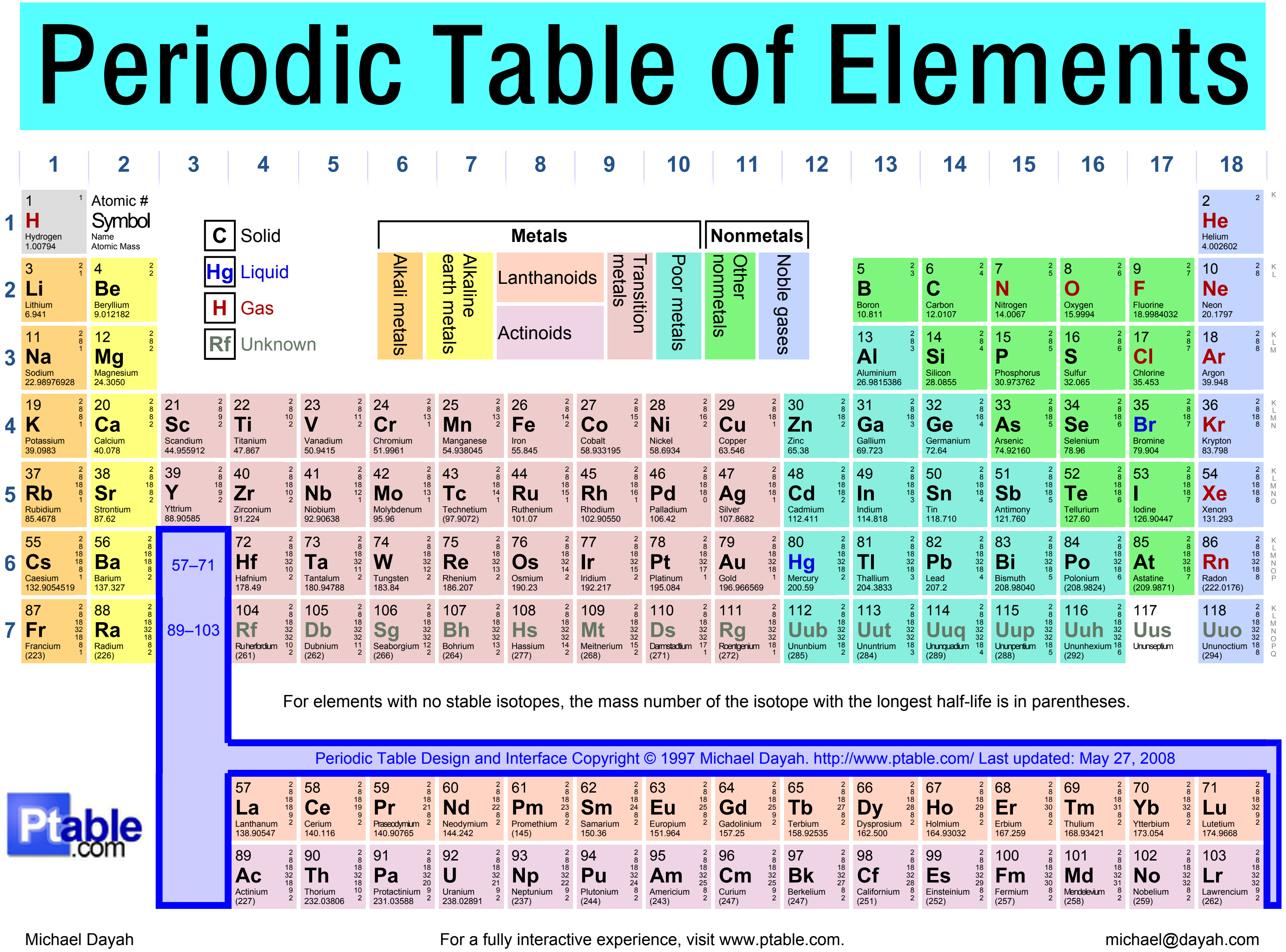
2. Multi-band model may be more appropriate starting point (definitely so if there is orbital degeneracy)

3. Spin-orbit interactions

4. (Obviously) must include long range Coulomb
+............................

In this lecture I will primarily consider situations in which many of these complications (mainly 1-3) are likely unimportant. Fortunately the cuprates fall in this class!

When Mott insulator?



Some classic Mott insulating materials: transition metal oxides (eg: NiO, MnO, V_2O_3, La2CuO4, LaTiO3,.......) of 3d series, some sulfides (NiS_2), ...

3d orbitals close to nucleus: large on-site repulsion compared to inter-site hopping.

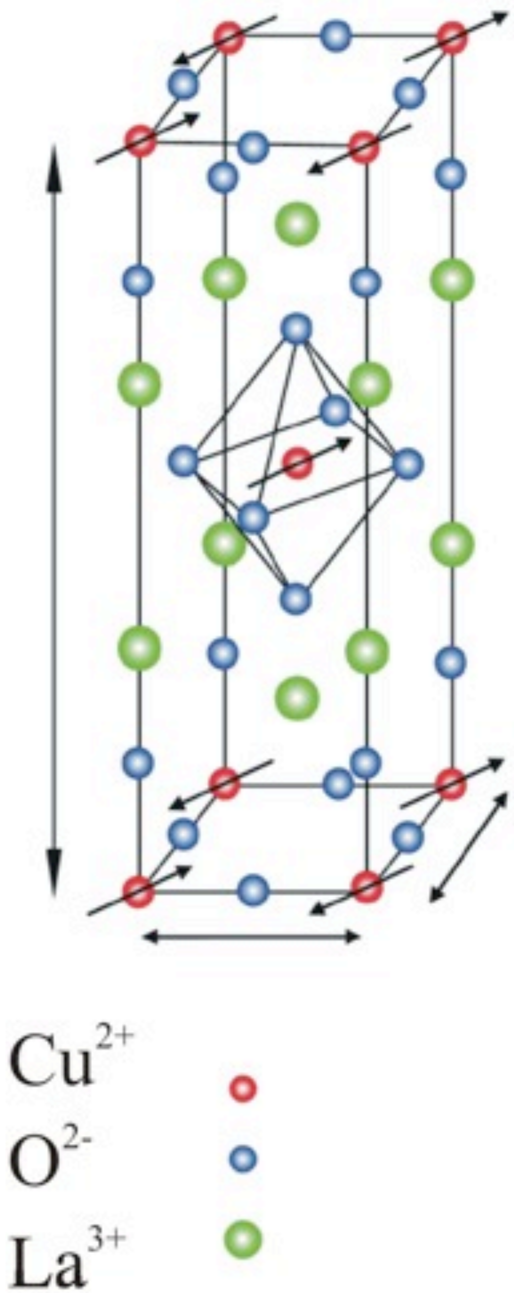
Will meet some other interesting examples later.

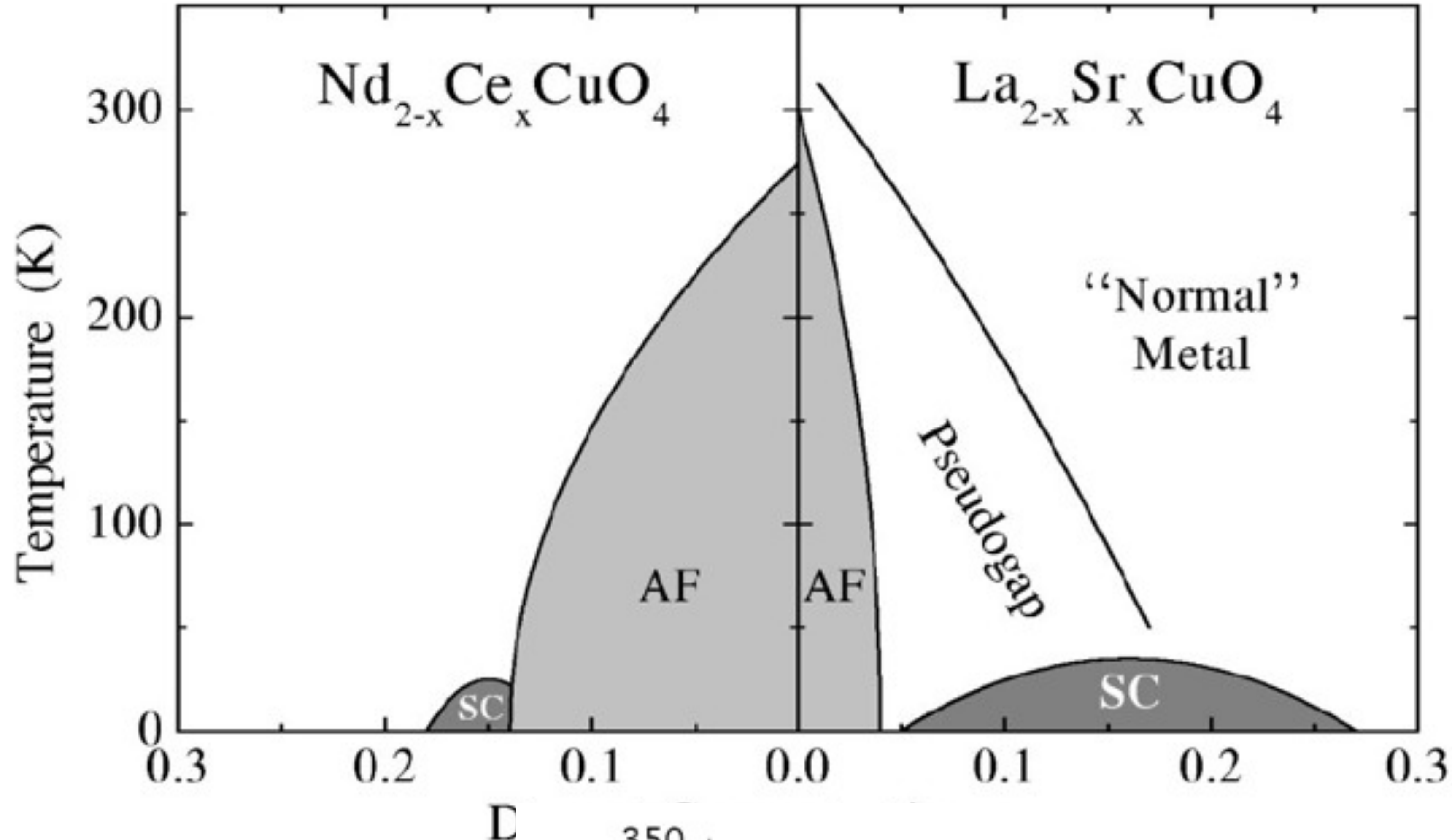
Recent additions: 5d transition metal oxides (eg: Sr2IrO4)

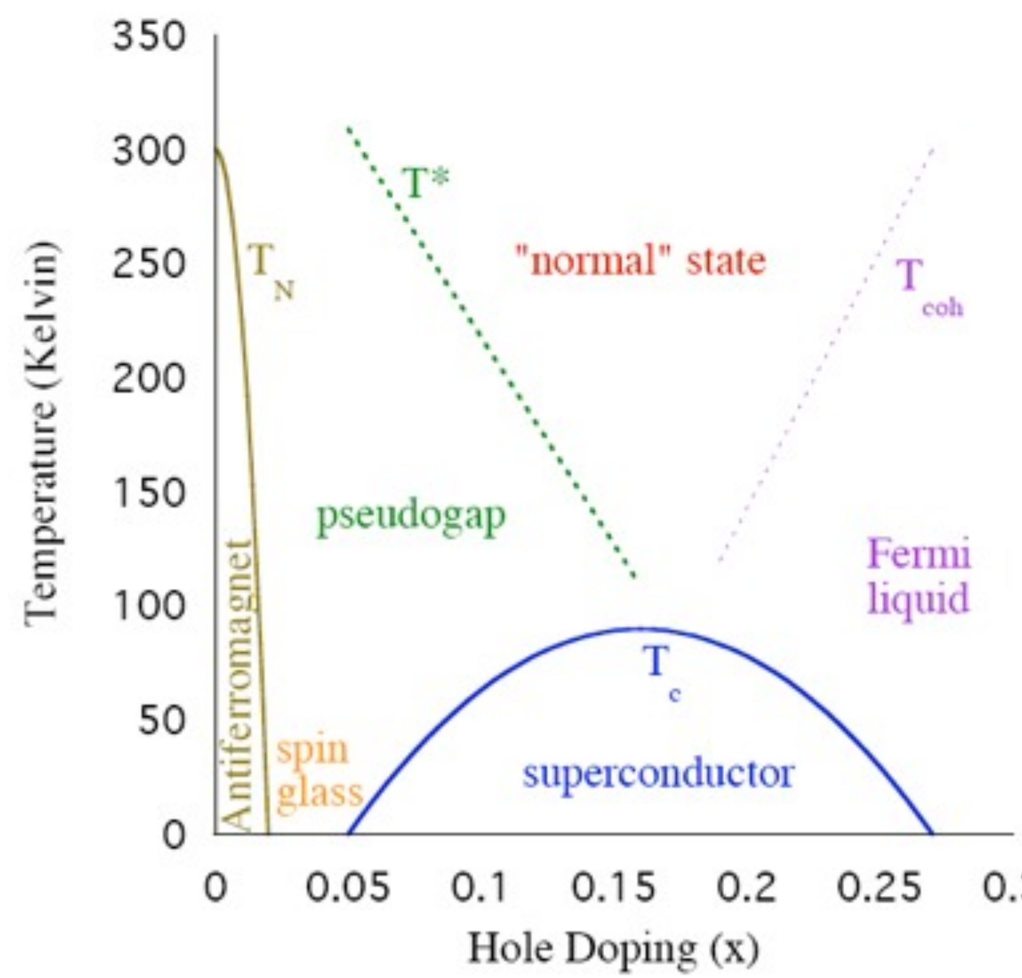
Atomic 5d orbitals more extended than 3d, 4d - so why Mott?

Mott insulation due to combination of strong spin-orbit + intermediate correlation.

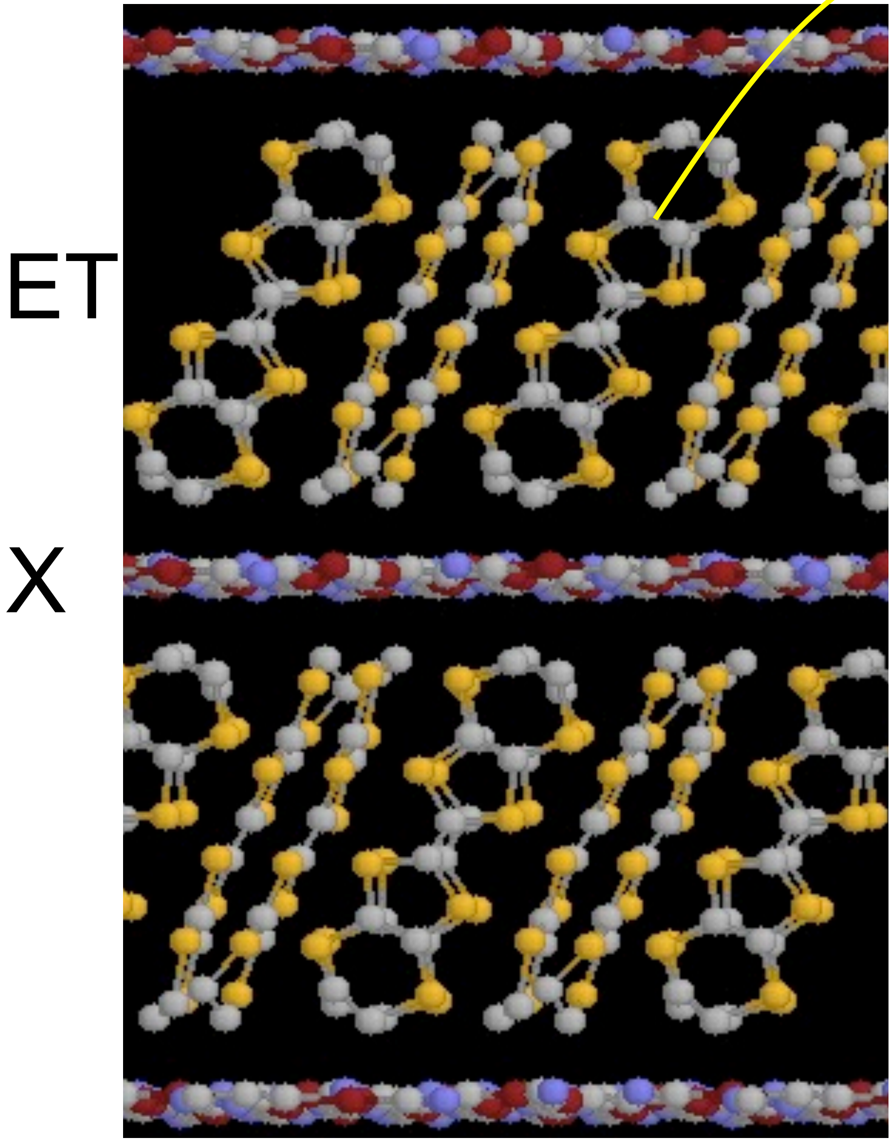
Many examples of superconductivity occurring in the vicinity of a Mott insulator.

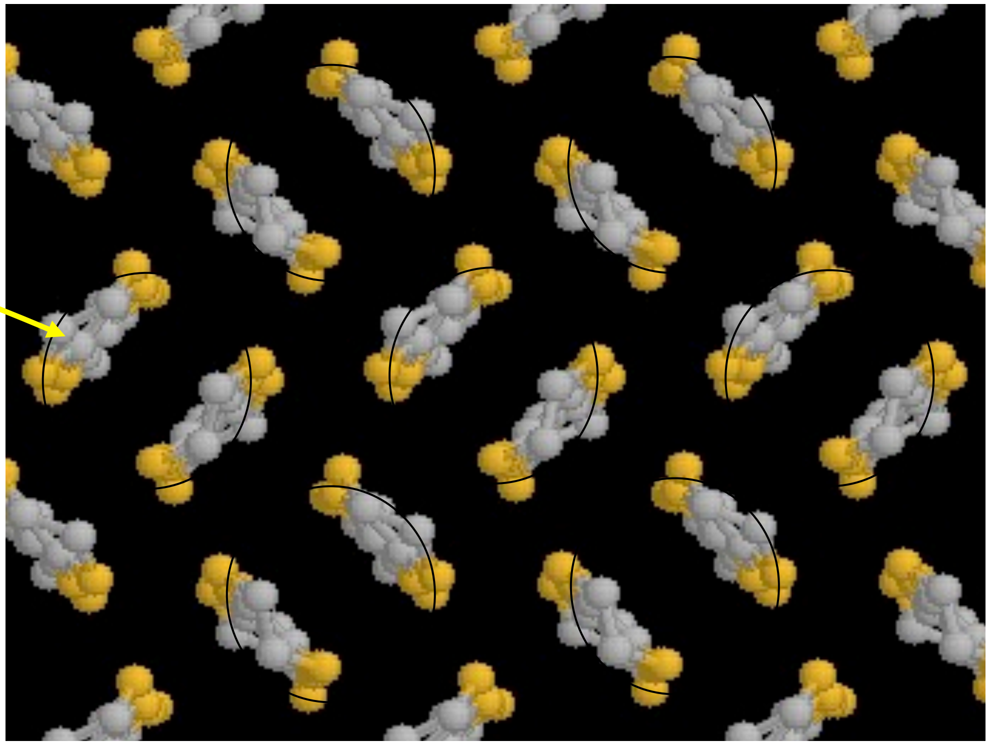

Cu^{2+}
O^{2-}
La^{3+}

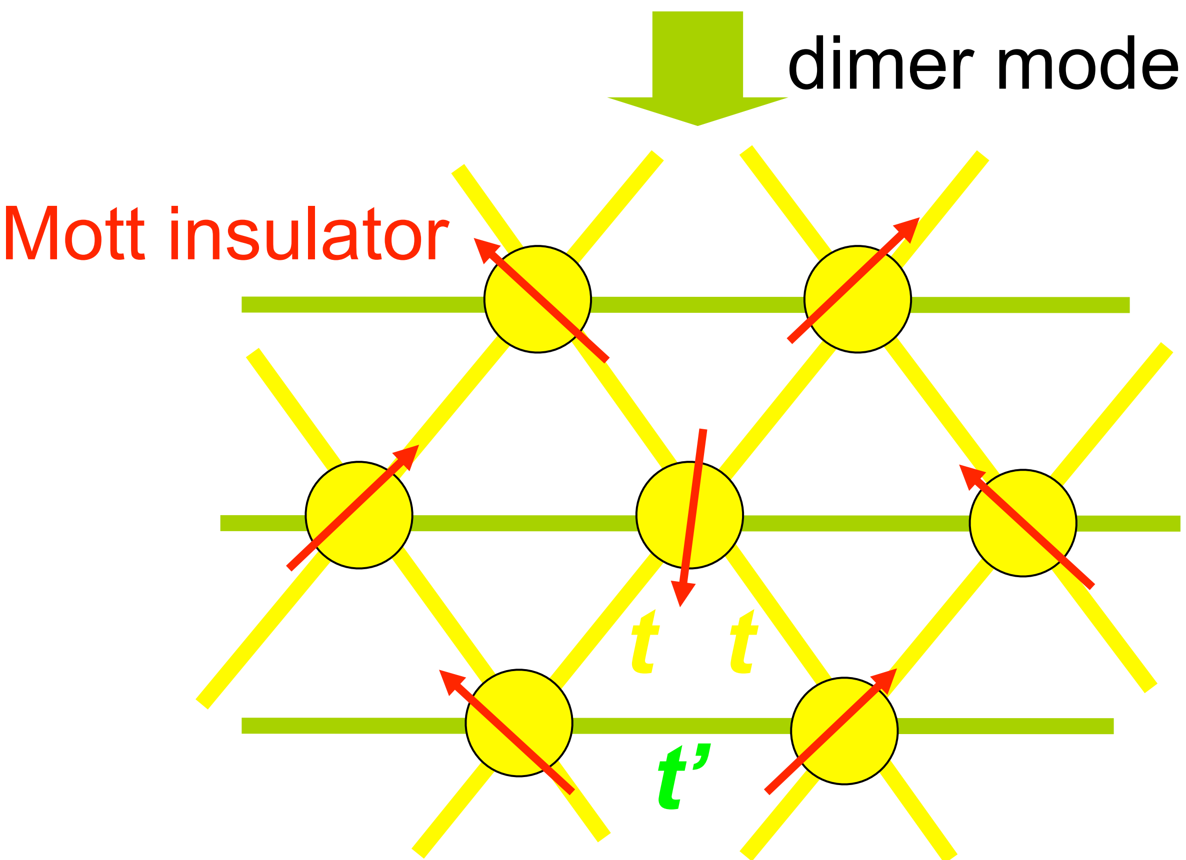

$Nd_{2-x}Ce_xCuO_4$
$La_{2-x}Sr_xCuO_4$
Temperature (K)
300
200
100
0
"Normal"
Metal
Pseudogap
AF
AF
SC
SC
0.3
0.2
0.1
0.0
0.0
0.1
0.2
0.3


Temperature (Kelvin)
350
300
250
200
150
100
50
0
T*
"normal" state
T_N
T_{coh}
pseudogap
Fermi
liquid
T_c
Antiferromagnet
spin
glass
superconductor
0
0.05
0.1
0.15
0.2
0.25
0.3
Hole Doping (x)

Quasi-2D organics κ-$(ET)_2X$





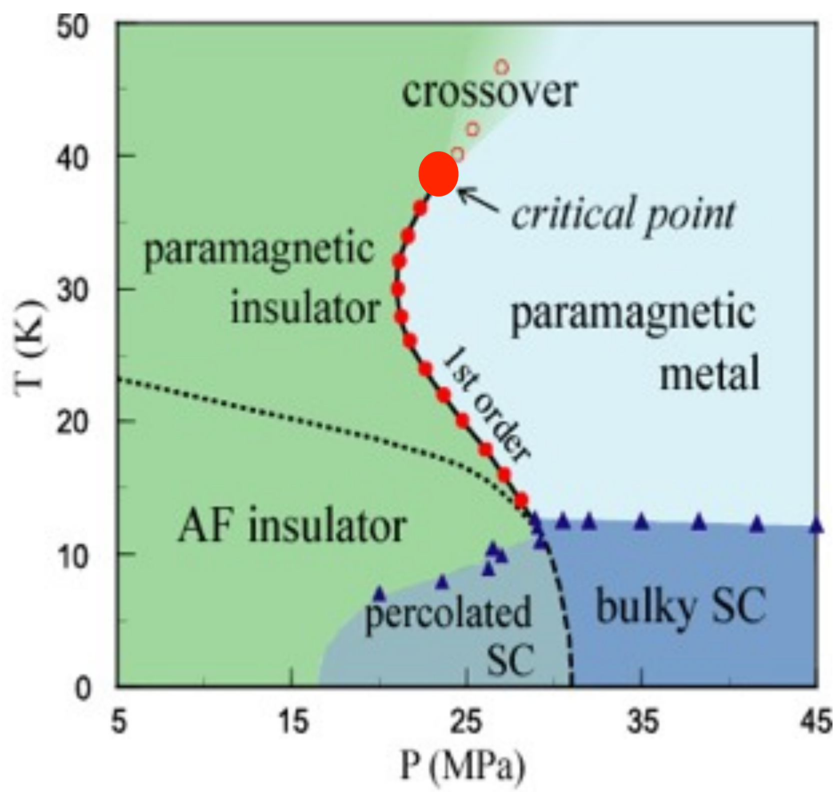


X = $Cu(NCS)_2$, $Cu[N(CN)_2]Br$, $Cu_2(CN)_3$…..

anisotropic triangular lattice

$t' / t = 0.5 \sim 1.1$

Pressure tuned superconductivity in the organics

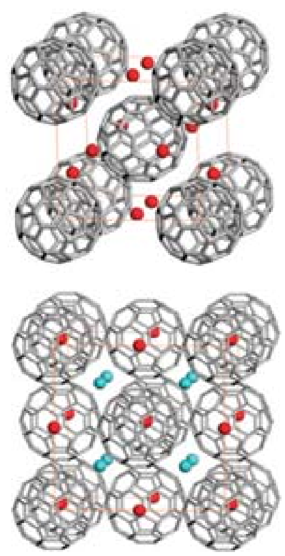


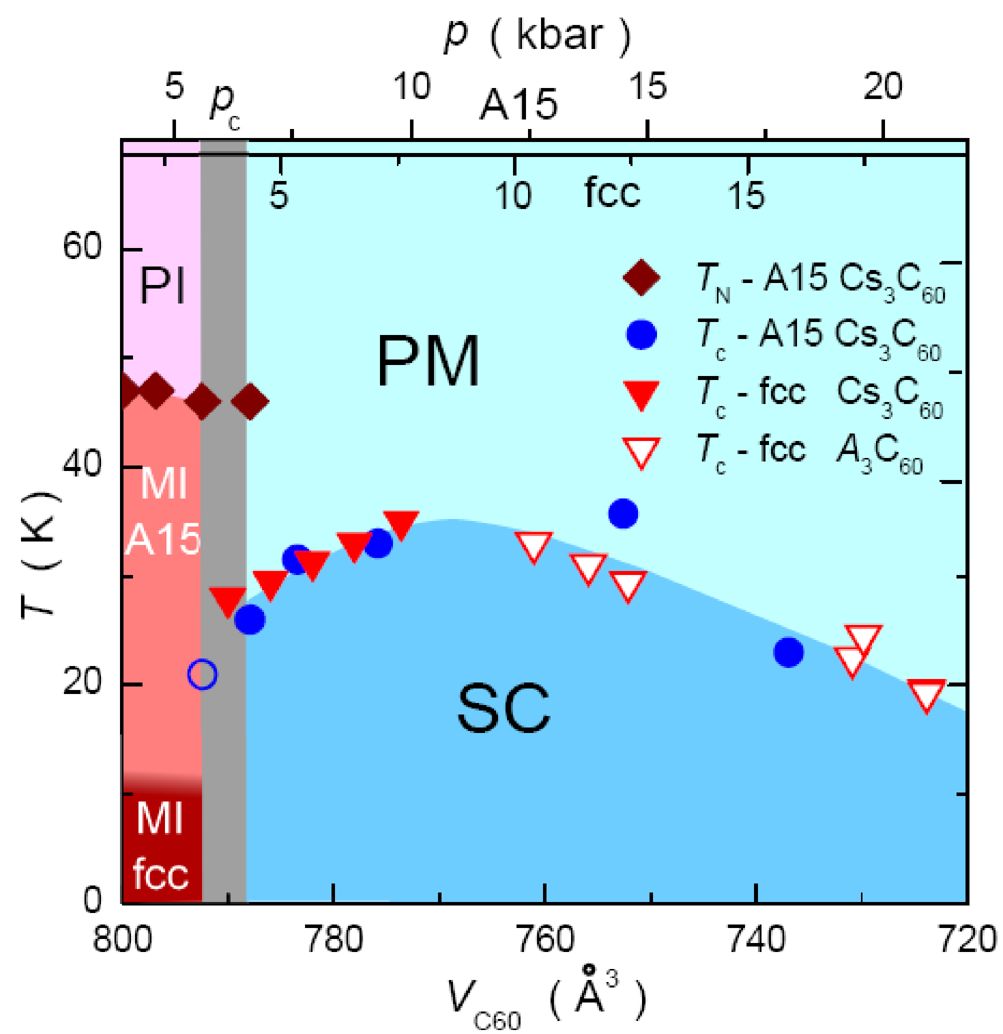
κ-Cu[N(CN)$_2$]Cl
t'/t = 0.75

Pressure decreases U/t.

Mott transition is induced by tuning U/t at fixed density of one electron per site.

Pressure tuned SC in fcc Cs3C60





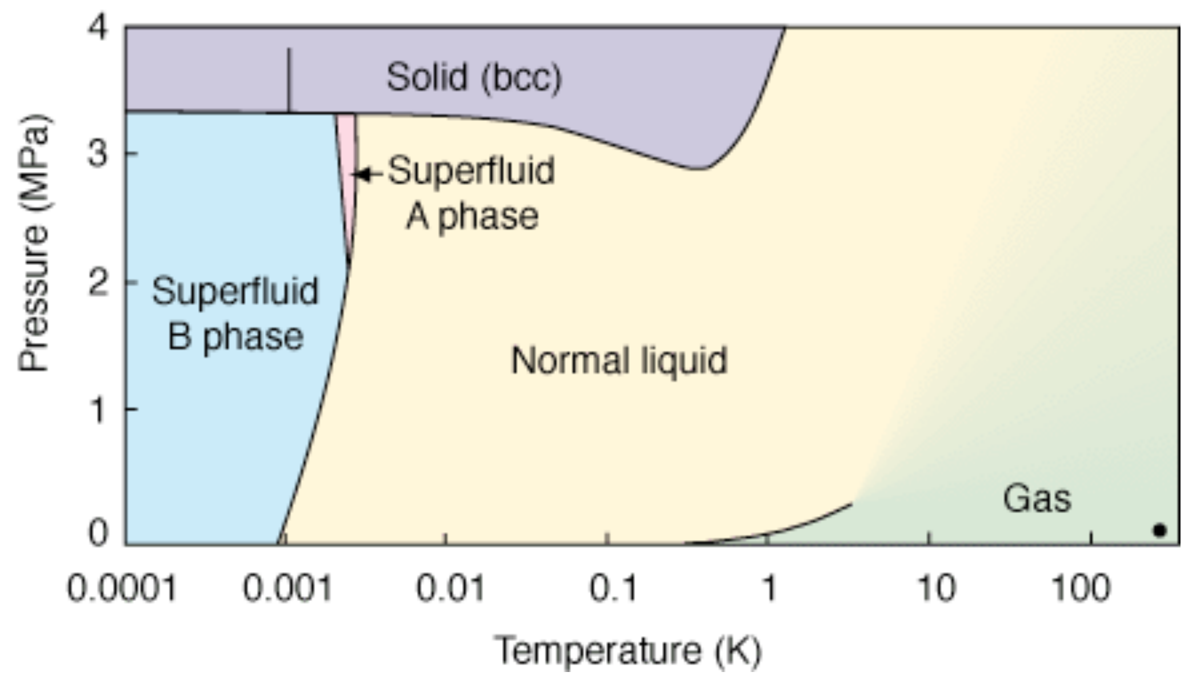
Ganin et al, Nature Materials, 2008, and Nature, 2010.

Ihara, Alloul, et al, PRL 2010.

Other related ??

Discussion question:

Superfluidity in He-3: `melted solid' fruitful point of view?



Solid ≈ Mott Insulator

Note that spin exchange scale of solid ≈ pairing scale in superfluid

Comments

Vicinity of the electronic Mott metal-insulator transition: many fascinating phenomena including but not limited to superconductivity.

0. Zeroth order fact: The metal-insulator transition itself !

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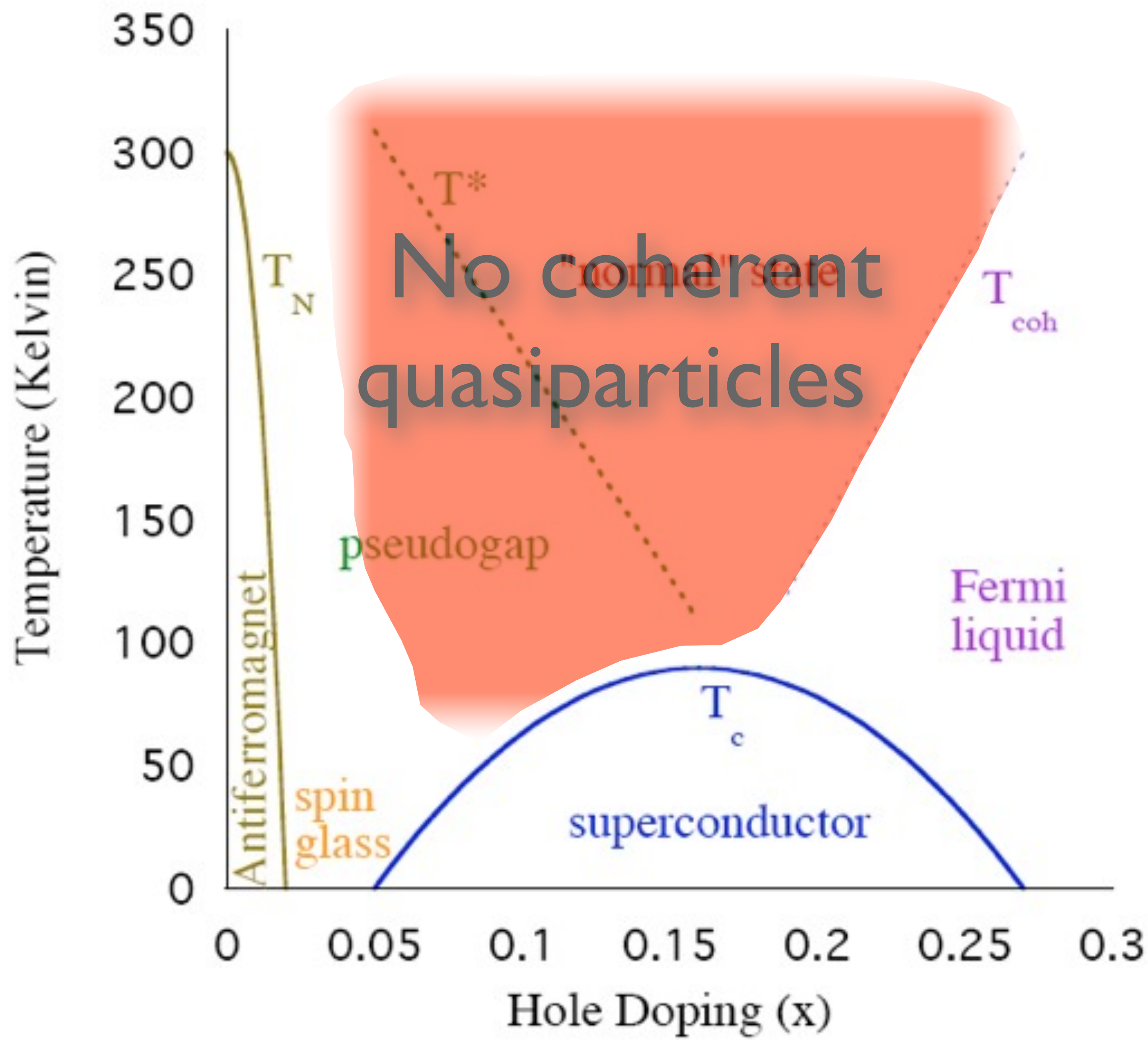
1. Emergence of strange metals

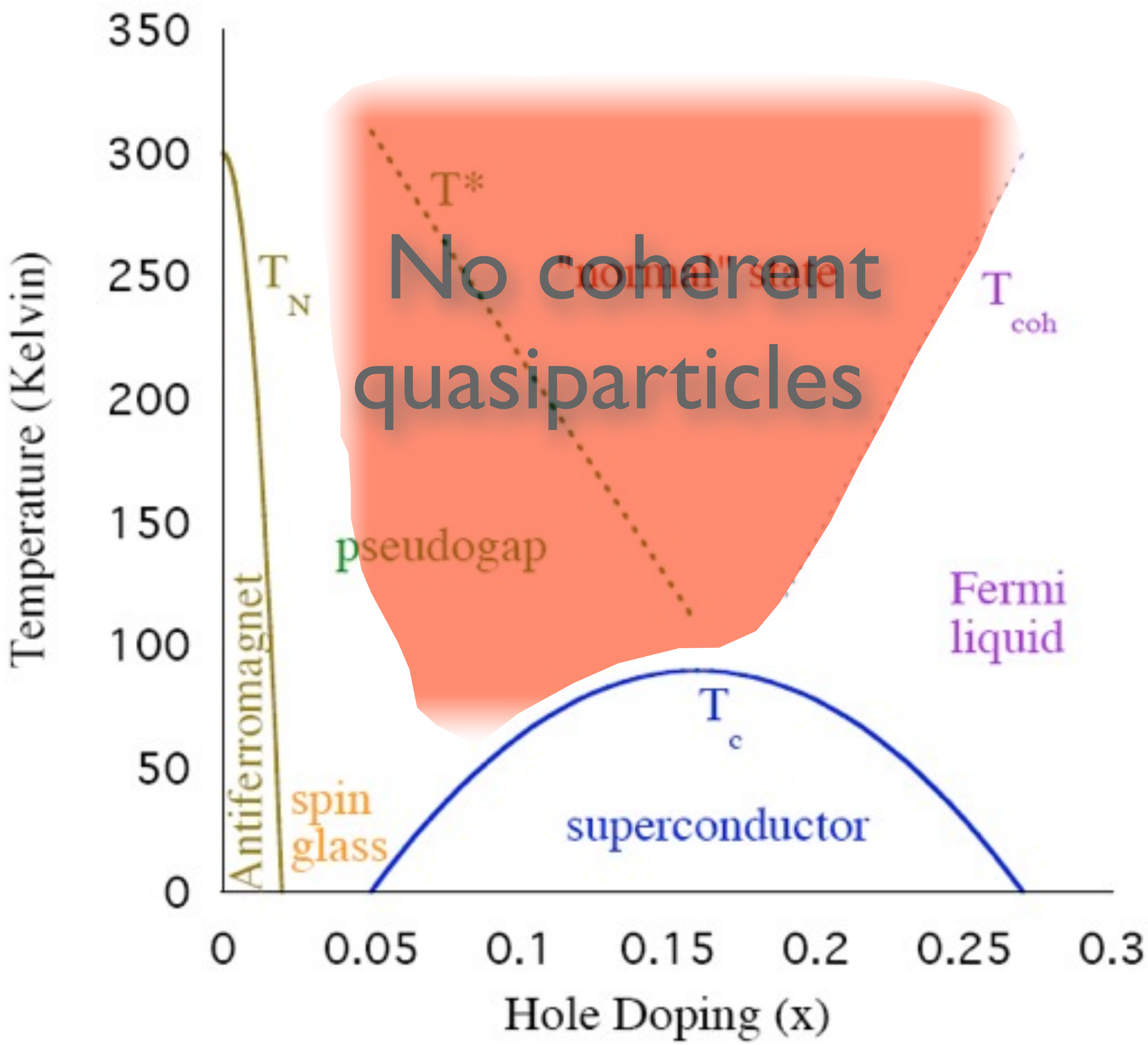
Coherent Landau quasiparticles emerge (if at all) at a low energy scale.

Example: cuprates



Coherent quasiparticles re-emerge in SC state.

Example: cuprates



Underdoped:

Across Tc two things happen.

1. Cooper pairs lose phase coherence

2. Electrons themselves also become incoherent

Discussion question: What really drives Tc in underdoped cuprates?

Conventional wisdom (Emery, Kivelson, 95): Low superfluid density
=> phase fluctuations of Cooper pair.

A more refined (alternate?) possibility:

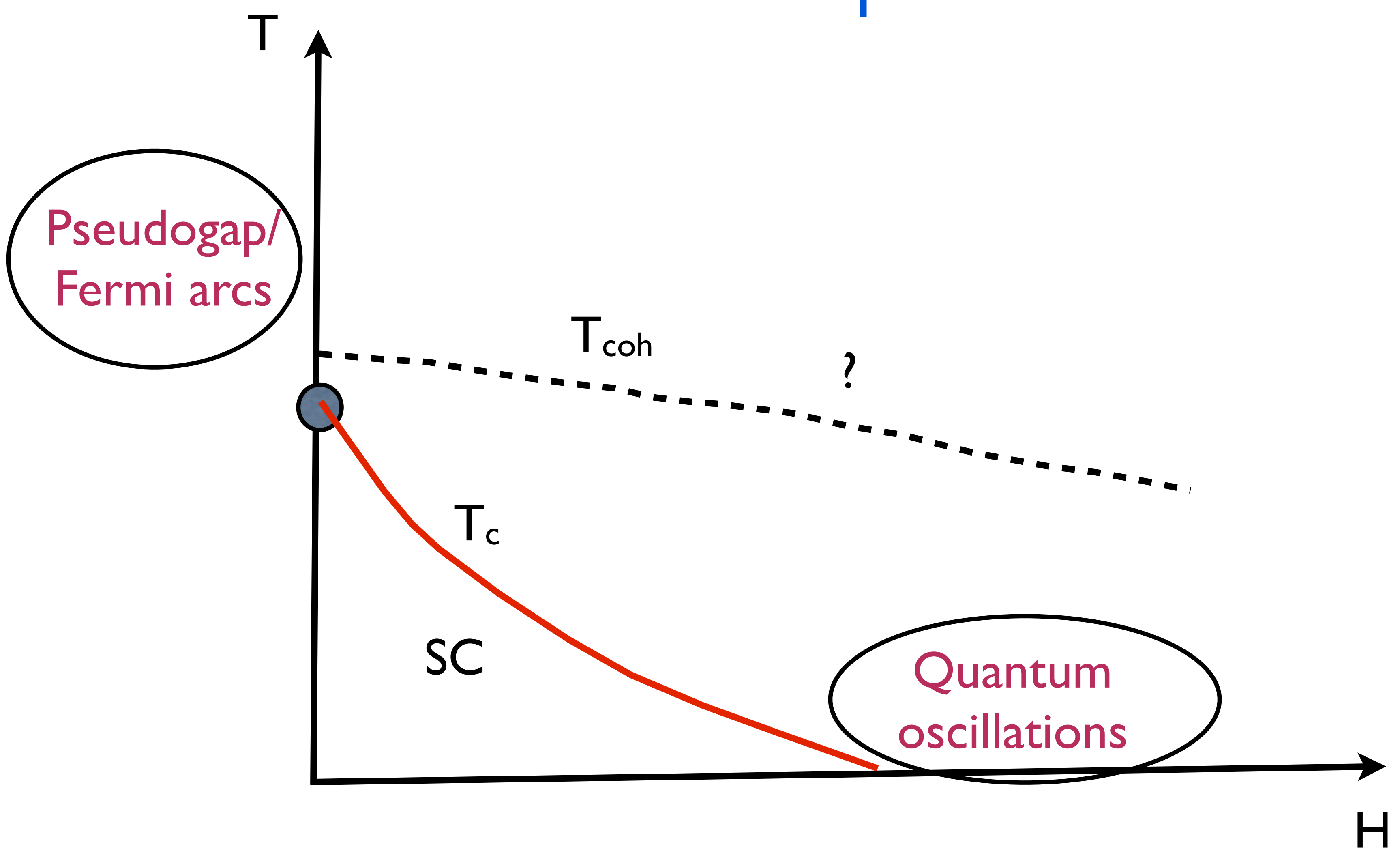
Incoherence of electron causes incoherence of Cooper pair.

Below electron coherence scale, Cooper pairs are able to condense.

Tc (and superfluid density) limited by low scale T_{coh} of single particle coherence.

Remark: effects of magnetic field on underdoped cuprate

TS, Lee, 2009



Explains why high T, low H $\neq$ low T, high H

H has suppressed T_c but not T_{coh} => reveals new regime not accessed by destroying SC by heating.

Comments

Vicinity of the electronic Mott metal-insulator transition: many fascinating phenomena including but not limited to superconductivity.

0. Zeroth order fact: The metal-insulator transition itself !

1. Emergence of strange metals

Coherent Landau quasiparticles emerge (if at all) at a low energy scale.

2. Other broken symmetry (eg, broken translation symmetry, electronic liquid crystals, ...) (see,eg, Randeria and Kivelson lectures)

3.. Emergence of strange insulators (see later).

SC near the Mott transition intertwined with many of these other phenomena.

Plan

Lecture 1

1. Examples of superconductivity and related phenomena near Mott transition

2. <u>**Magnetism and Mott insulators**</u>

Briefly discuss general nature of magnetism in Mott insulators

Lecture 2

Metals and superconductors near the Mott transition

-(i) some general questions
-(ii) some theoretical answers.

Magnetism and Mott insulators

Prototype: ½-filled Hubbard model at large-U

$$H = -\sum t_{ij} \left(c^{+}_{i\alpha} c_{j\alpha} + h.c \right) + U \sum_i \frac{n_i (n_i - 1)}{2}$$

Large-U : Charges localize below some temperature $\sim o(U)$

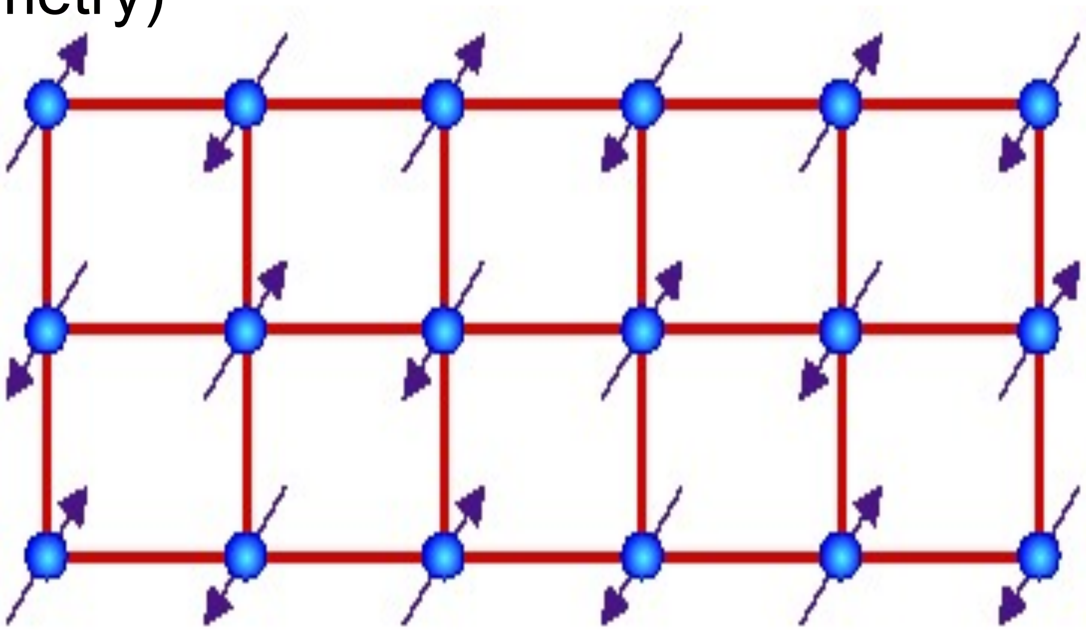
Active low energy degree of freedom is electron spin

Describe by $H_{eff} \approx J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + \ldots\ldots$

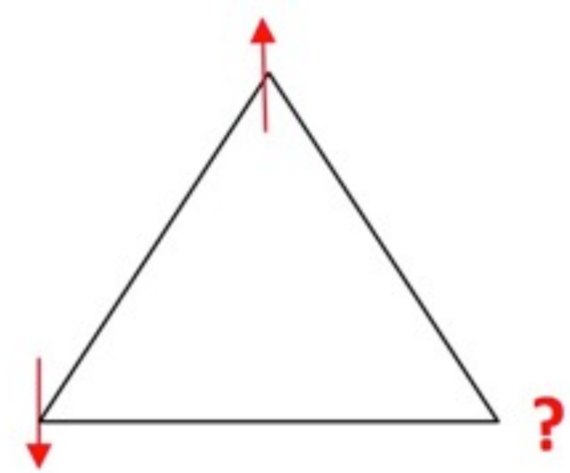
$\left(J \sim t^2/U > 0 \right)$

Fate of electron spins in a Mott insulator

Common: Neel Antiferromagnetism (spontaneously breaks global spin SU(2) symmetry)

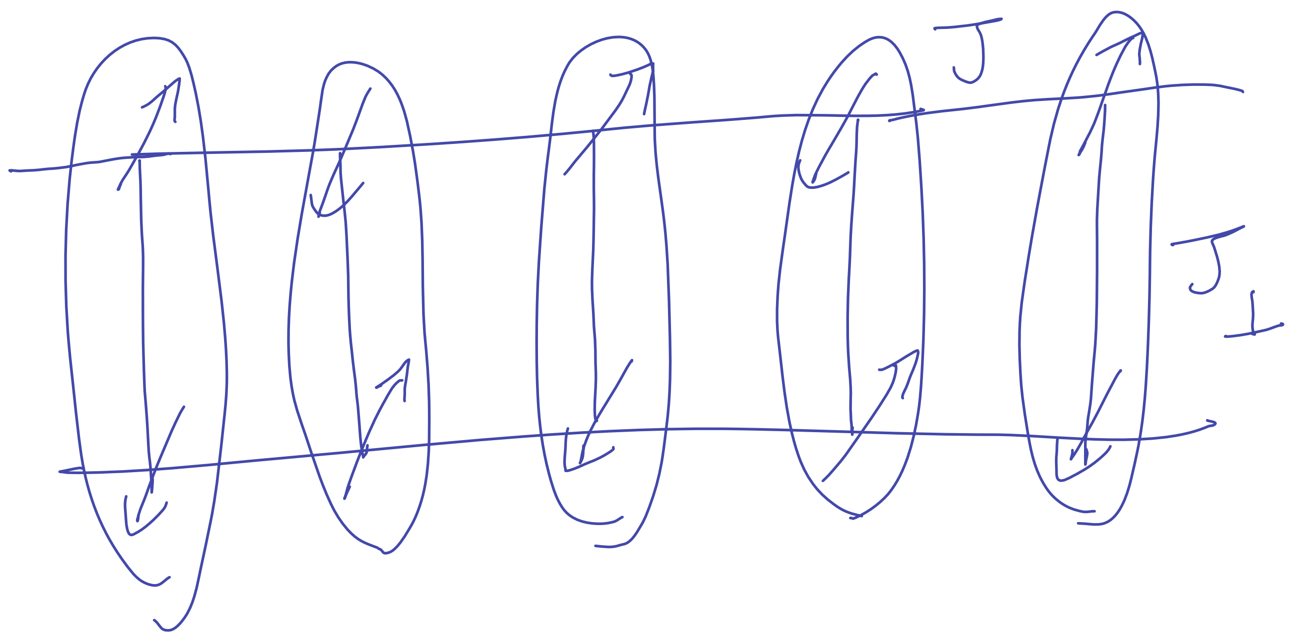


Interesting situations with low dimension/quantum fluctuations/``geometrically frustration"



Can get states that preserve spin SU(2) symmetry to T = 0 (``quantum paramagnets")

Spin ladders: A simple example of a quantum paramagnet



$J_\perp \gg J$:

Form rung singlets

$\Rightarrow$ Paramagnetic ground state

Smoothly connected to $J_\perp \ll J$!

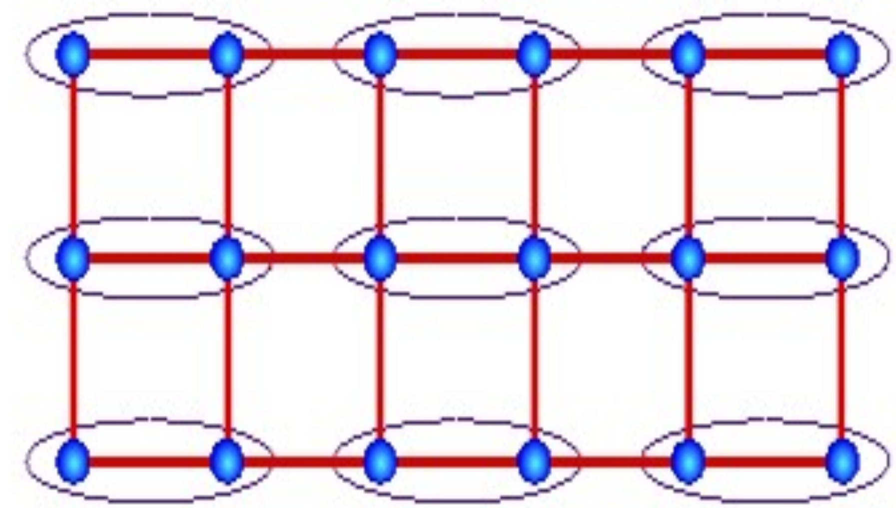
Many examples ($SrCu_2O_3$, . . .)

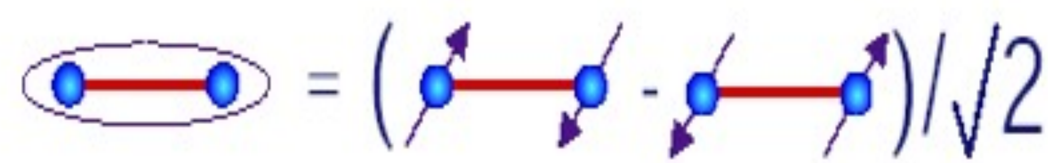
Other quantum paramagnets: ``Spin-Peierls”/Valence Bond Solid(VBS) states

- Ordered pattern of valence bonds breaks lattice translation symmetry.

- Ground state smoothly connected to band insulator

- Elementary spinful excitations have S = 1 above spin gap.





Seen in many model calculations (Eg: Sandvik J-Q model on square lattice)

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - Q \sum_{\langle ijkl \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right) \left(\vec{S}_k \cdot \vec{S}_l - \frac{1}{4} \right)$$

Materials: CuGeO3, TiOCl, some organic salts, ...

Most interesting possibility: quantum spin liquids

What is a quantum spin liquid?

Rough definition: Quantum paramagnet which does not break any symmetries.

Better rough definition: Mott insulator with ground state not smoothly connected to band insulator.

Best definition: Mott insulator with ***``long range quantum entanglement”*** in ground state.

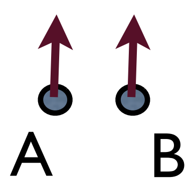
(Important) Digression

Non-local quantum entanglement in macroscopic matter

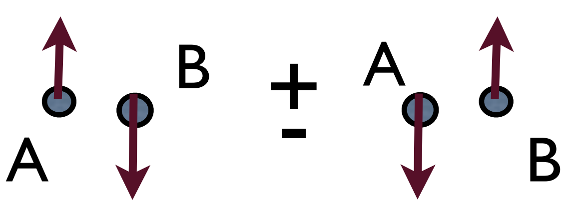
Entanglement in quantum mechanics

Two parts A and B of a quantum mechanical system may be ``entangled'' with each other.

Example: Spin orientations of two electrons in a simple molecule



unentangled; each spin by itself in a definite quantum state

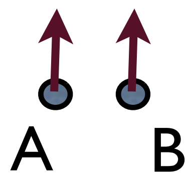


entangled: each spin by itself not in a definite quantum state though full system is.

I would not call entanglement ***one*** but rather ***the*** characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought.

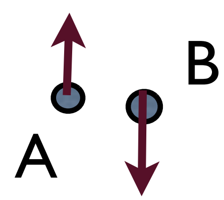
E. Schrodinger, 1935

The relation of a part to the whole

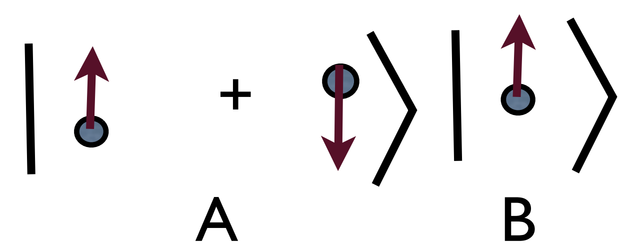


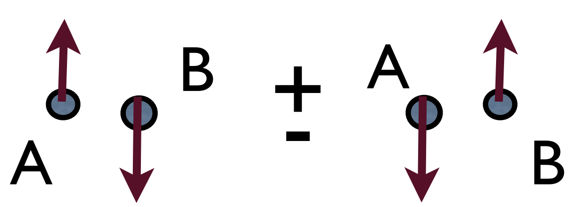
Unentangled parts: wavefunction of whole system factorizes into a product of wavefunctions of parts.

Other examples:



or even



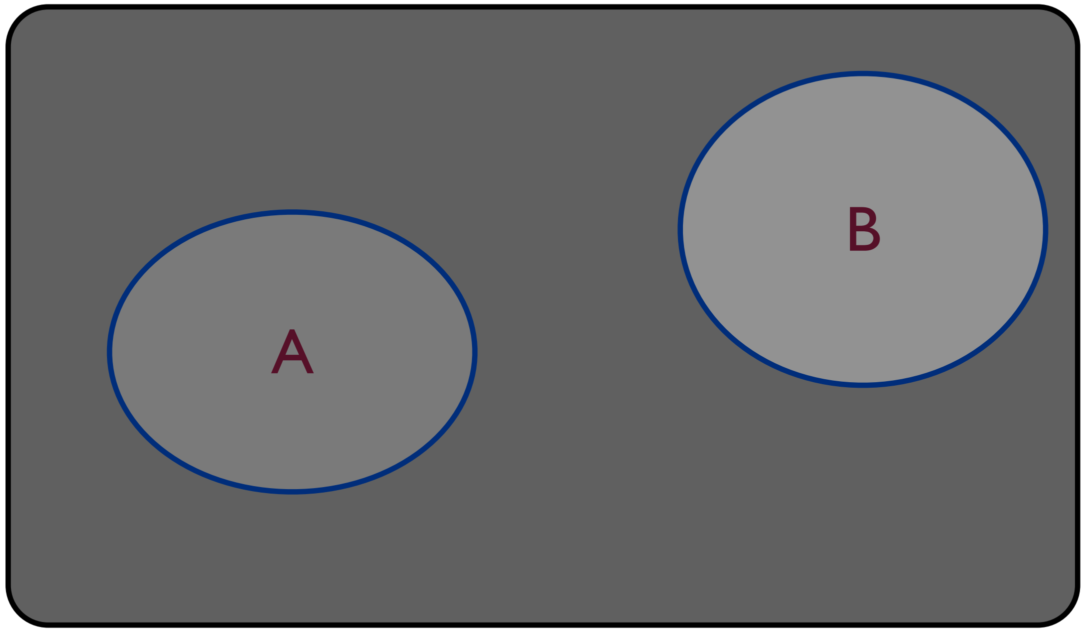


Entangled parts: Wavefunction of full system does not factorize as products of wavefunction of parts.

Cannot describe one part fully without the other.

Entanglement and macroscopic matter

How are the different parts of a piece of macroscopic matter entangled quantum mechanically with each other?



A deep and fundamental question.........

Importance only became clear in last few years.

Very fruitful in our ongoing attempt to characterize distinct phases of quantum matter.

Entanglement between A and B?

Phases of matter

Macroscopic matter in equilibrium organizes itself into phases.

Solids, liquids, gases.......

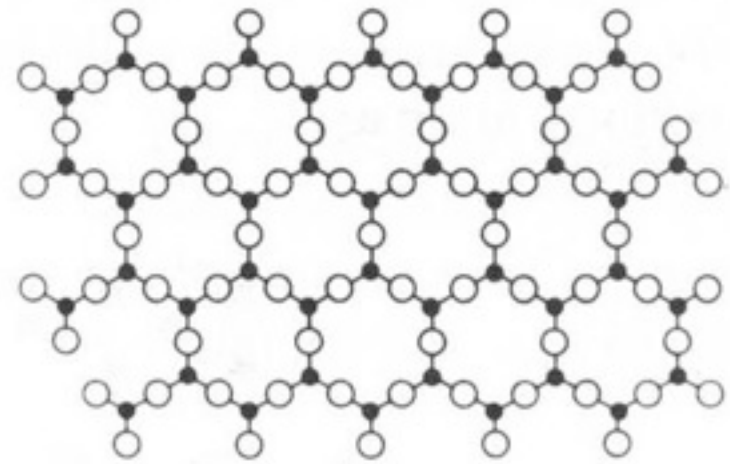
Magnets........

Superconductors.............

Organizing principles: long range order and broken symmetry

Example: crystalline solid.

Atoms arrange themselves into an ordered array.



Pattern of atomic positions in one region determines atomic positions far away.

Broken symmetry: Microscopic interactions invariant under translating all atoms but equilibrium state is not.

General consequences of broken symmetry

Pattern of broken symmetry determines many macroscopic properties of ordered matter.

Examples: rigidity of solids, persistence of currents in a superconductor, etc.

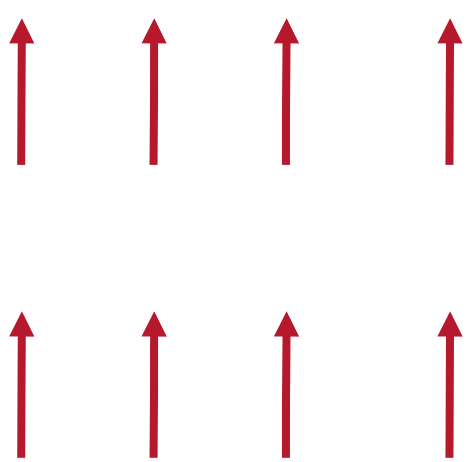
Broken symmetry point of view: unifying theoretical framework for many seemingly distinct properties of matter.

Magnetism: an illustrative example

Most familiar form of magnetism: ferromagnetism.

Discovered may be around 600 BC.

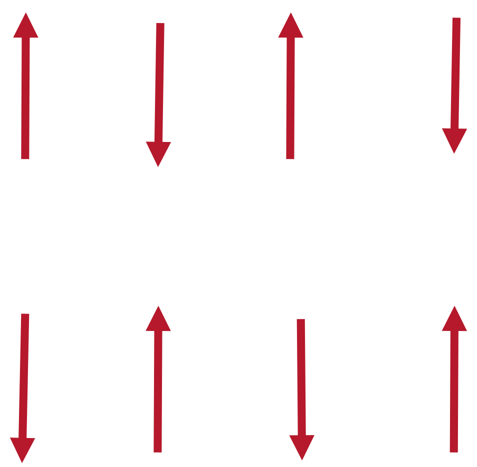
Microscopic picture: Electron spins inside magnet are all pointed in same direction.



Example of broken symmetry: Microscopic interactions do not pick direction for spin but macroscopic magnetized state has specific spin orientation.

Antiferromagnetism: The more common magnetism

Actually the more common form of magnetism is
not ferromagnetism but antiferromagnetism.



Also a broken symmetry state -
spin orientation frozen in time but oscillates in space
Microscopic interactions allow any orientation.

Despite being more common antiferromagnetism was
discovered only in the 1930s!

Ferromagnetism: easily detected.

Antiferromagnetism: need microscopic probes that sense
spin orientation with atomic spatial resolution.

Quantum description of magnetism

The essential properties of these magnetic states of matter is contained in their ground state wavefunction.

Example: Prototypical wavefunctions

Ferromagnet $|\uparrow\uparrow\uparrow\uparrow \cdots\cdots\cdots\rangle$

Antiferromagnet $|\uparrow\downarrow\uparrow\downarrow \cdots\cdots\cdots\rangle$

Prototypical wavefunctions capture the pattern of broken symmetry which holds the key to many macroscopic properties of these phases.

Short range entanglement

For familiar magnetic states,
prototypical ground state wavefunction factorizes as
direct product of local degrees of freedom

$$|\uparrow\uparrow\uparrow\uparrow \cdots\cdots\cdots\rangle$$

$$|\uparrow\downarrow\uparrow\downarrow \cdots\cdots\cdots\rangle$$

Quantum entanglement short ranged in space.

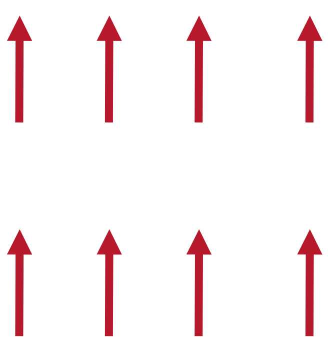
1930s- present: elaboration of broken symmetry and other states with short range entanglement

Emergence of classical physics

Broken symmetry states of magnetism:

Macroscopic description in terms of classical physics of the ``thing'' that orders.

Example: spontaneous magnetization of a ferromagnet.



Microscopic quantum spins

Macroscopic classical magnet

Modern times

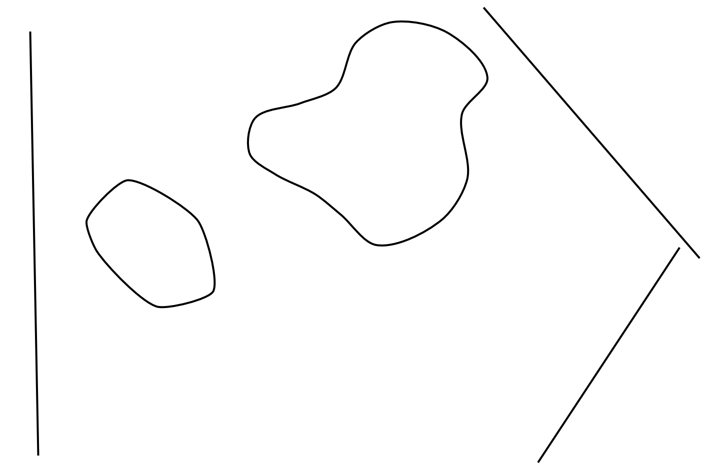
Discovery of a *qualitatively* new kind of magnetic matter.

Popular name: ``quantum spin liquid”

Prototypical ground state wavefunction

Not a direct product of local degrees of freedom.

Quantum entanglement is long ranged in space.



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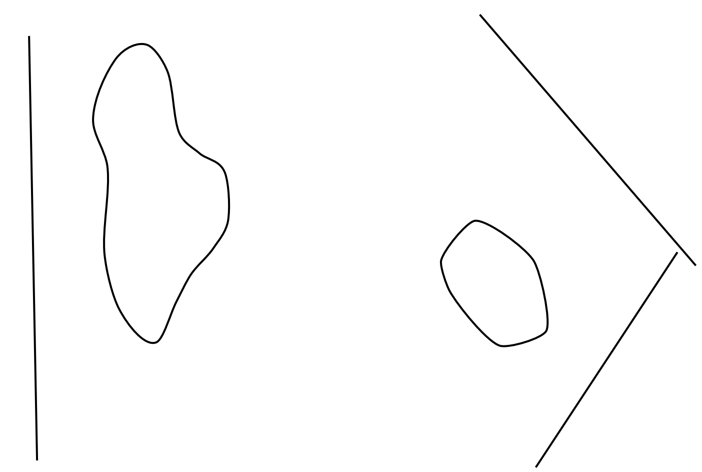
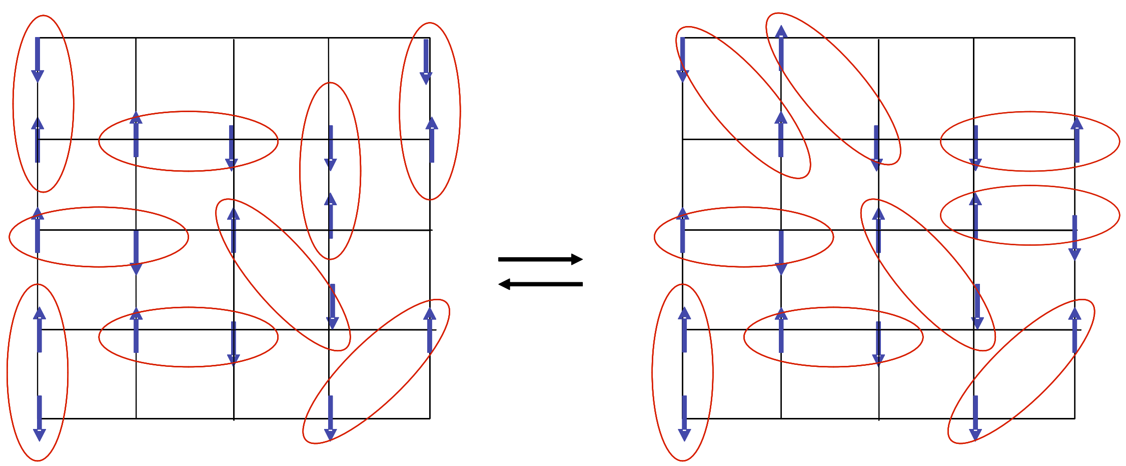


+ ....

* In d > 1

What is a quantum spin liquid?

Rough description: Spins do not freeze but fluctuate in time and space due to quantum zero point motion.



Resonance between many different configurations (like in benzene)
In each configuration each spin forms an ***entangled pair*** with one other partner spin.

Envisaged by P.W. Anderson (1973, 1987);

Long Range Entangled (LRE) phases

Universal information about state not visible by looking only at small local part of system.

Passage from microscopic to macroscopic scales - classical physics does not emerge.
(contrast with broken symmetry phases, eg, ferromagnet)

Older very famous example: Fractional quantum Hall states.

Other fascinating examples:
Conventional metals: ``Fermi Liquid" state (oldest familiar Long Range Entangled state)

Many new metals: ``Non-fermi liquids"

Can quantum spin liquid phases exist?
Question for theory

Yes!!! (work of many people over last 25 years)

Many dramatic phenomena seen to be theoretically possible.

Examples:

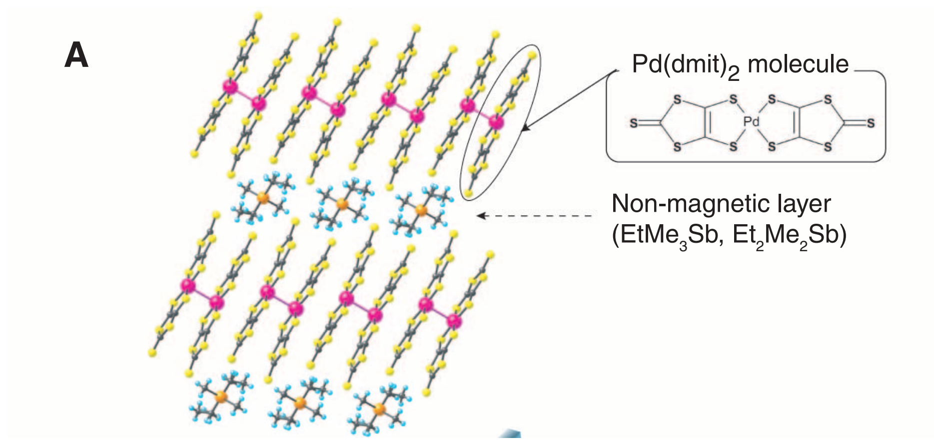
1. Electron can break apart into fractions

2. Emergence of long range quantum mechanical interactions between fractional pieces of electron.

Similar phenomena established in FQHE in two dimensions in strong magnetic fields but now are known to be possible in much less restrictive situations.

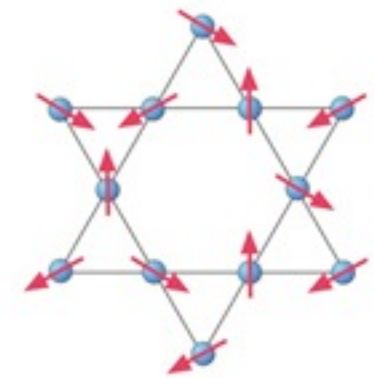
Do quantum spin liquid phases exist?
Question for experiment

Yes - many interesting candidate materials in last few years!!



Layered organic crystals $\kappa-(ET)_2Cu_2(CN)_3$ Kanoda et al, 2003-now

$EtMe_3Sb[Pd(dmit)_2]_2$ Kato et al, 2008



Some layered inorganic minerals

$ZnCu_3(OH)_6Cl_2$ (Y. Lee, Nocera et al, 2007)

Herbertsmithite

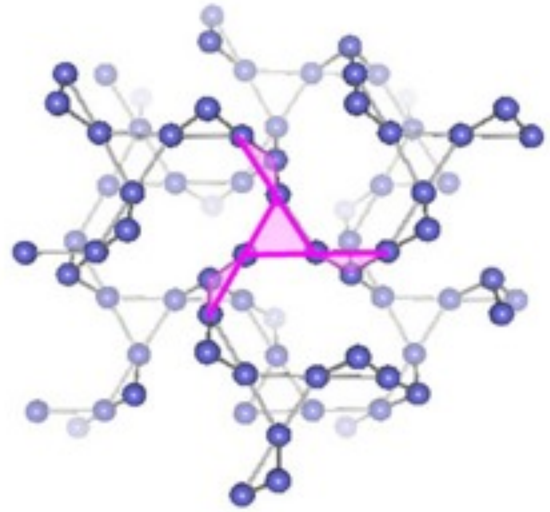
$Cu_3V_2O_7(OH)_2 \cdot 2H_2O$ (Z. Hiroi et al, 2010)

Volborthite

Three dimensional transition metal oxide

$Na_4Ir_3O_8$

(H. Takagi et al, 2008)



Some phenomena in experiments

Quantum spin liquid materials are all electrical insulators.

Despite this many properties other than electrical conduction are very similar to that of a metal.

Two examples at low temperature:

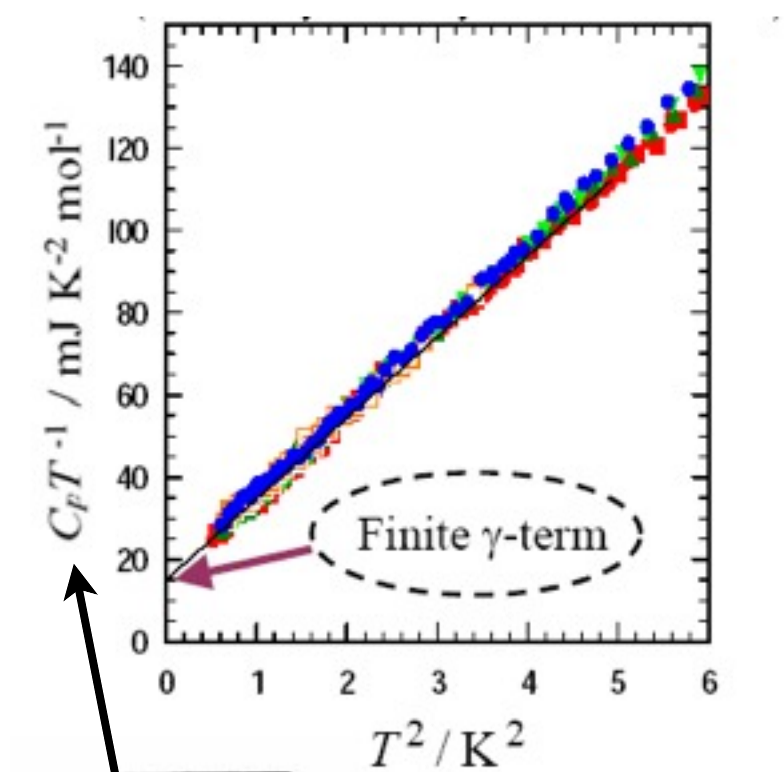
1. Entropy very similar to that of a metal at low temperature

2. Conduct heat just like a metal even though they are electrical insulators.

Very strange......not known to happen in any ordinary insulator.

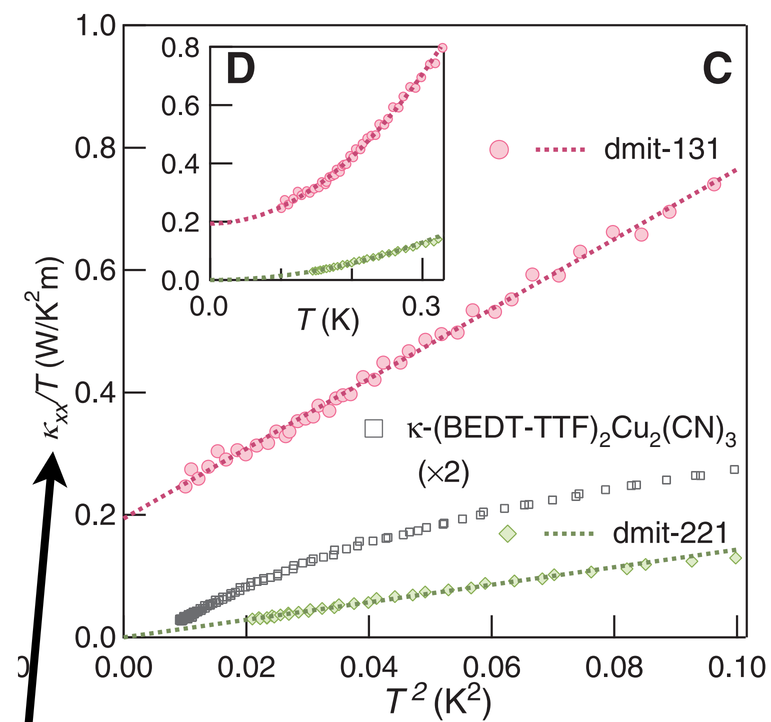
Some phenomena in experiments

S. Yamashita et al, Nat Phys, 2008



Heat capacity

M.Yamashita et al, Science 2010



Thermal conductivity

These are both exactly like in a metal but were measured in an insulator.

Towards understanding experiments

Low-T properties of metals are determined by mobile electrons obeying Pauli exclusion principle.

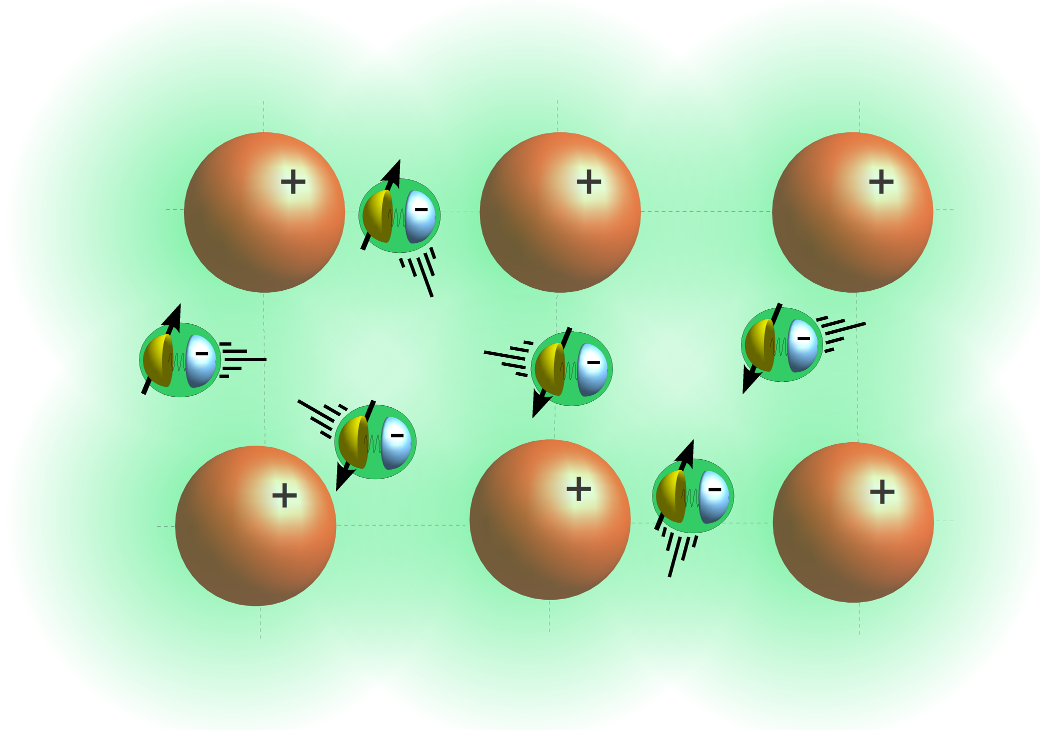
In an insulator there cannot be mobile electrons.

A promising idea: perhaps there are emergent particles obeying Pauli exclusion that carry the electron spin but not its charge inside these materials.

Such phenomena are known to be theoretically possible in LRE phases (but are prohibited if there is only SRE)

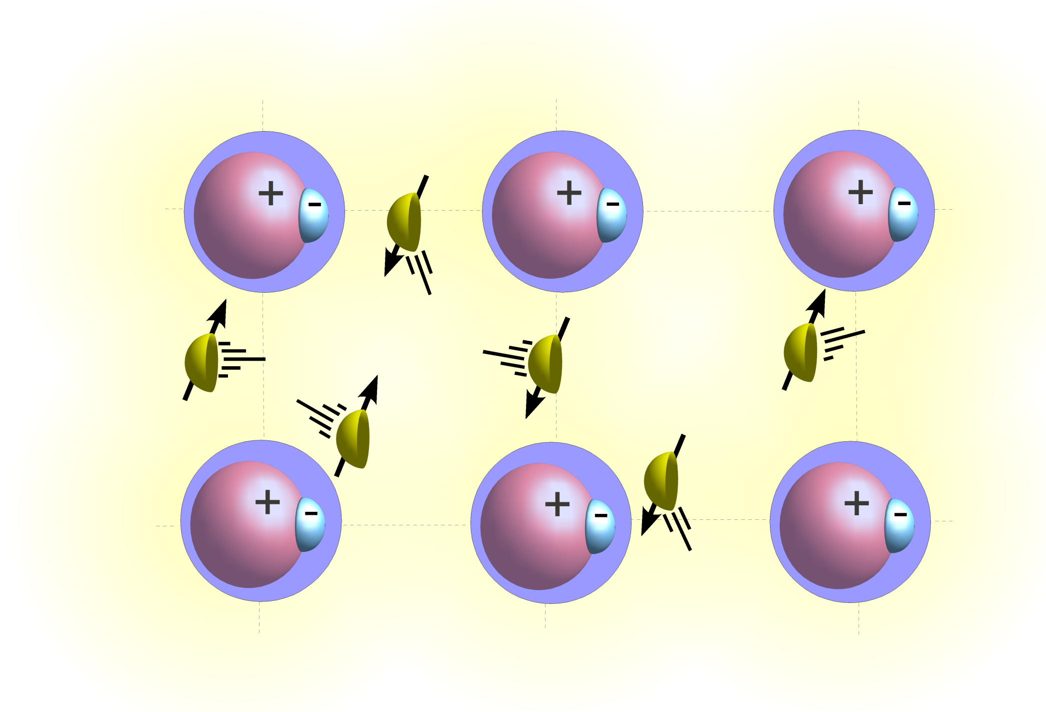
Picture of a particular quantum spin liquid

Metal



Electrons swimming in sea of +vely charged ions

A quantum spin liquid



Electron charge gets pinned to ionic lattice while spins continue to swim freely.

Future prospects: short term

1. Combined theory/experiment effort to characterize currently existing quantum spin liquids.

??Directly demonstrate non-local entanglement in experiment??

2. Theory predicts possibility of wide variety of such exotic phases of magnetic matter.

Future prospects: long term

In the last 3 decades, growing number of experimental discoveries* have dethroned all the ``textbook'' paradigms of the old field of solid state physics.

Some of these we understand; most of these we do not.

Our eyes have been opened to a new ***truly quantum*** world of 10^{23} electrons.

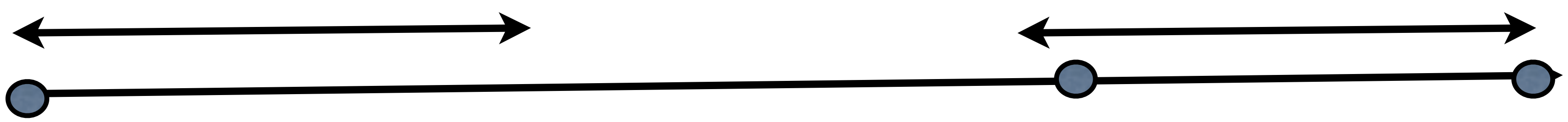
Characterizing ``***pattern of entanglement***'' in macroscopic quantum matter promises to be as rich and profound as the previous century's efforts at characterizing broken symmetry.

*FQHE (1982), high temperature superconductivity (1987), strange metals where electron-like charge carriers do not exist, quantum spin liquid magnets

Entanglement and Phases of quantum matter

``Short range entangled”

``Long range entangled”



Conventional
phases
Eg: Band insulators,
superfluids/
superconductors,
antiferromagnets,
....

Gapped
`topologically ordered’
phases
Eg: FQHE

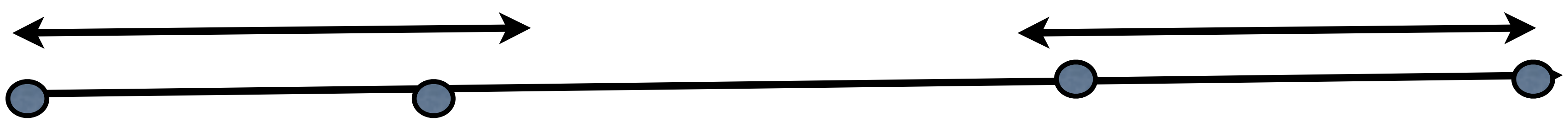
Gapless* phases/critical
points
Eg: Fermi/ non-fermi liquids

*Not just Goldstone

Entanglement and Phases of quantum matter

``Short range entangled"

``Long range entangled"



Conventional phases
Eg: Band insulators, superfluids/ superconductors, antiferromagnets,
....

Almost conventional phases: Topological insulators

Gapped `topologically ordered' phases
Eg: FQHE

Gapless phases/critical points
Eg: Fermi/ non-fermi liquids

End of digression

Remarks

A wide variety of distinct kinds of quantum spin liquid phases can exist - distinct physical properties and low energy effective field theories.

A gross distinction: Gapped versus gapless

Gapped spin liquids - many interesting properties (topological order, etc); not the focus here.

Gapless spin liquids: relevant to experiments and as a platform for understanding emergence of metal/superconductors near the Mott transition.

A useful theoretical framework

Slave particle construction $\vec{S}_r = \frac{1}{2} f^{\dagger}_{r\alpha} \frac{\vec{\sigma}_{\alpha\beta}}{2} f_{r\beta}$

$f_{r\alpha}$: fermionic 'spinon' with spin α.

Constraint $f^{\dagger}_r f_r = 1$ ensures physical Hilbert space.

Redundant description, e.g., can let $f_{r\alpha} \to e^{i\theta_r} f_{r\alpha}$.

Full redundancy: $SU(2)$ gauge transformation

A useful theoretical framework (cont'd)

Strategy: Put f in some mean field state with a quadratic Hamiltonian.

Examples:

1. 'spinon metal'

$$H_{MF} = -t_f \sum_{rr'} f_r^\dagger f_{r'} + h.c$$

Spin physics similar to metal

2. 'Paired'

$$H_{MF} = -t_f \sum_{rr'} f_r^\dagger f_{r'} + \Delta_{rr'}(f_{r\uparrow} f_{r'\downarrow} - f_{r\downarrow} f_{r'\uparrow}) + h.c$$

Spin physics similar to superconductor

Mean field theory for highly non-trivial quantum spin liquid insulators

Fluctuations

Mean field Hamiltonian breaks gauge redundancy down to a subgroup.

Fluctuations beyond mean field: must couple f to gauge fields in that subgroup.

Effective field theory: spinon + fluctuating gauge fields.

Use to address stability (`lower critical dimension', etc) and predict testable physical properties.

Example:

1. `Spinon metal':

Spinon Fermi surface + fluctuating U(1) gauge field.

2. Paired spin liquid

Spinons + fluctuating Z_2 gauge field.

A physical description:
Quantum spin liquids near the Mott transition

Start with the metal.

Interacting Fermi fluid: Incorporate correlations with Jastrow factor

$$\psi_F(\mathbf{r}_1\sigma_1, ...\mathbf{r}_N\sigma_N) = \prod_{ij} f(\mathbf{r}_i - \mathbf{r}_j)\psi_{Slater}(\mathbf{r}_1\sigma_1, ...\mathbf{r}_N\sigma_N) \quad (1)$$

Special case: Gutzwiller approximation to lattice Hubbard model choose

$$f_{ij} = g\delta_{ij} \quad (2)$$

with $g < 1$ to weigh down double occupancy of any site.

Can think of $f(\mathbf{r}_i - \mathbf{r}_j)$ as wave function of a boson fluid.
Boson coordinates are slaved to electrons.

Quantum spin liquids near the Mott transition

Wavefunction of insulator:
Replace $f(\mathbf{r}_i - \mathbf{r}_j)$ by wave function of boson insulator ψ_{BI}

$$\psi_F = \psi_{BI}\psi_{Slater}$$

ψ_{BI} suppresses charge fluctuations.
Extreme case: Remove all charge fluctuation - Gutzwiller projection P_G to no double occupancy to get spin wave function.

$$\psi_{SL} = P_G\psi_{Slater}$$

Can repeat with BCS wavefunction instead of Slater for the `paired' spin liquid.

Wavefunctions closely connected to those from slave particle approach.

Though quantum paramagnets may exist the cuprate (and many other) Mott insulators are actually antiferromagnetically ordered.

Nevertheless it will be useful to consider the emergence of metals and superconductors from various kinds of Mott insulators, not just antiferromagnets.

Doping a quantum spin liquid

Spinon metal → Fermi Liquid

Paired spin liquid → Superconductor.

Wavefunctions:

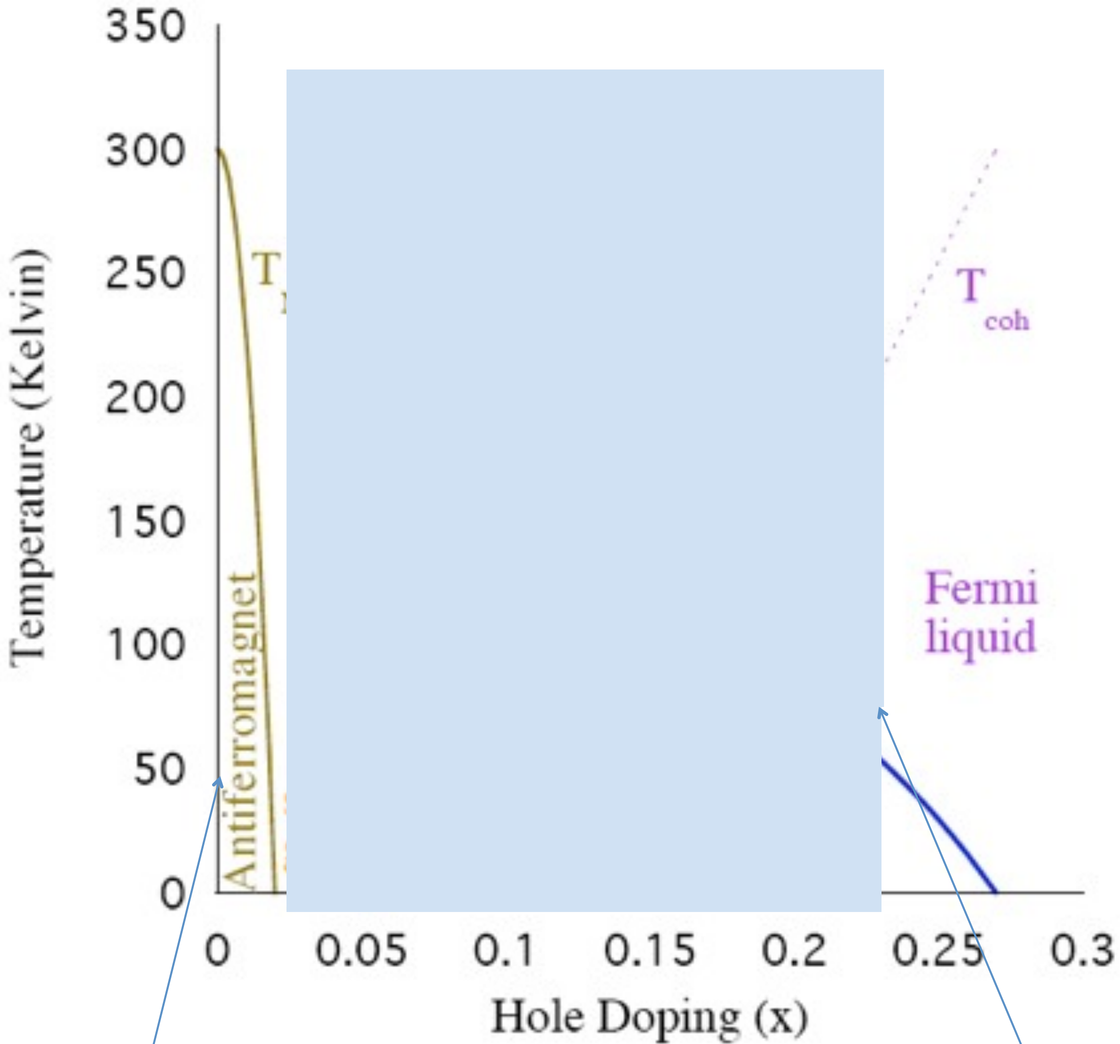
Doped spinon metal $\psi = P_G \psi_{Slater}$ (now not at half-filling)

Wavefunction of (correlated) Fermi liquid.

Doped paired spin liquid $\psi = P_G \psi_{BCS}$

Wavefunction of (correlated) superconductor.

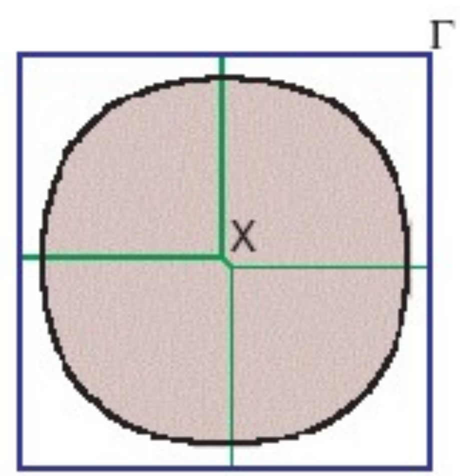
High Tc cuprates: how does a Fermi surface emerge from a doped Mott insulator?



Evolution from Mott insulator to overdoped metal : emergence of large Fermi surface with area set by usual Luttinger count.

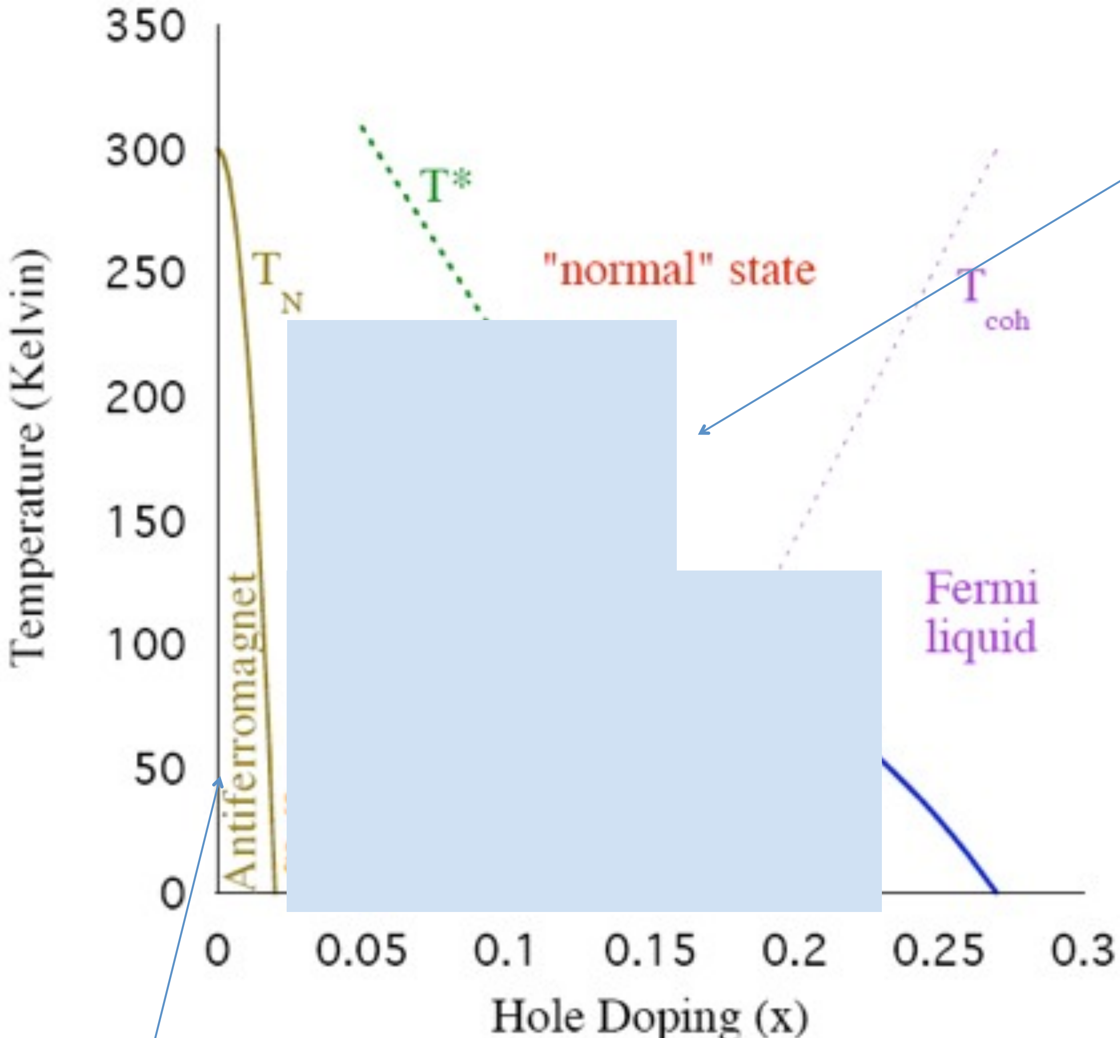
Mott insulator:
No Fermi surface

Overdoped metal:
Large Fermi surface



ADMR, quantum oscillations (Hussey), ARPES (Damascelli,....)

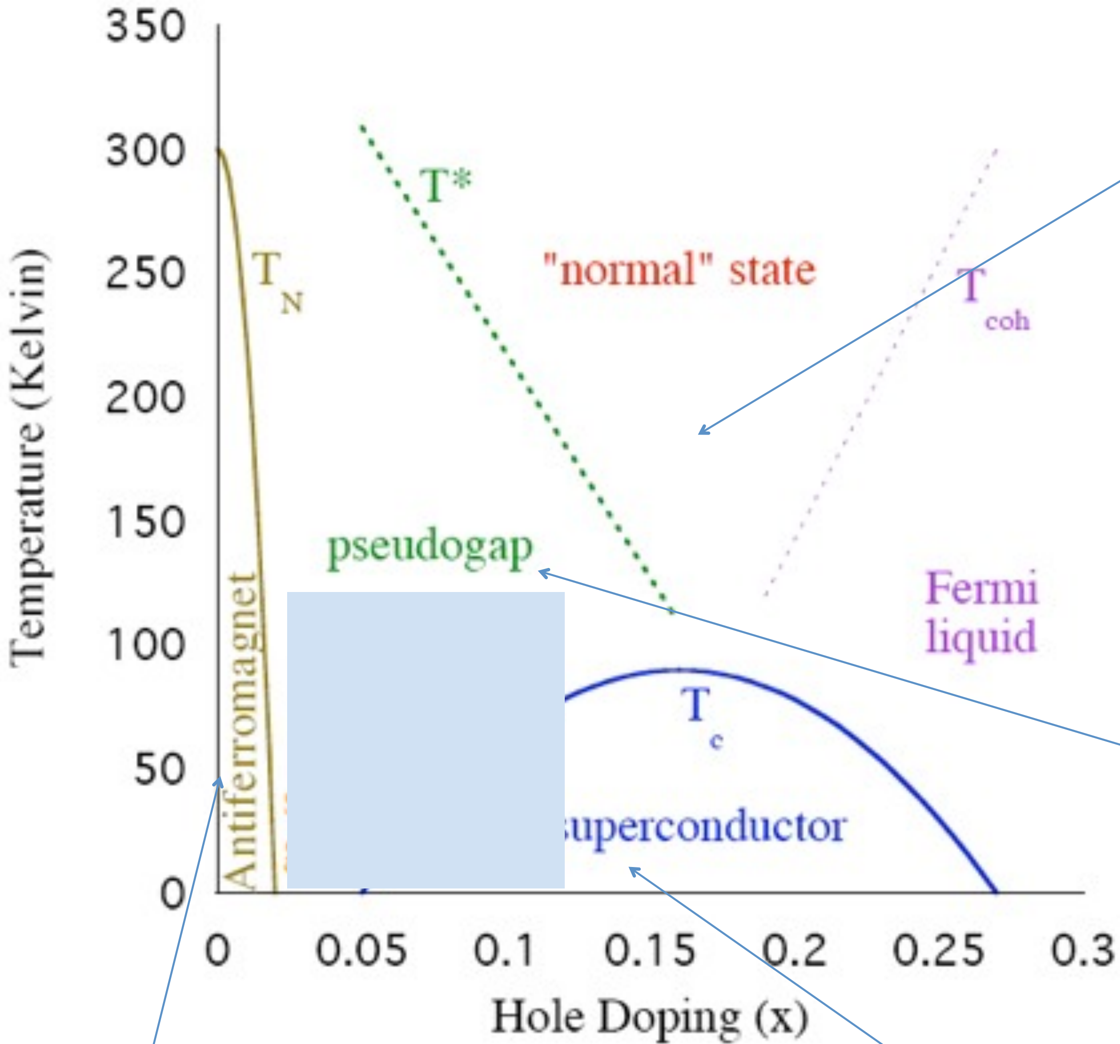
High Tc cuprates: how does a Fermi surface emerge from a doped Mott insulator?



Large gapless Fermi surface present even in optimal doped strange metal albeit without Landau quasiparticles .

Mott insulator:
No Fermi surface

High Tc cuprates: how does a Fermi surface emerge from a doped Mott insulator?



Large gapless Fermi surface present also in optimal doped strange metal albeit without Landau quasiparticles .

Even in the pseudogap regime the minimum gap features (nodal Fermi arcs, antinodal gaps) in ARPES are apparently located at large Fermi surface!

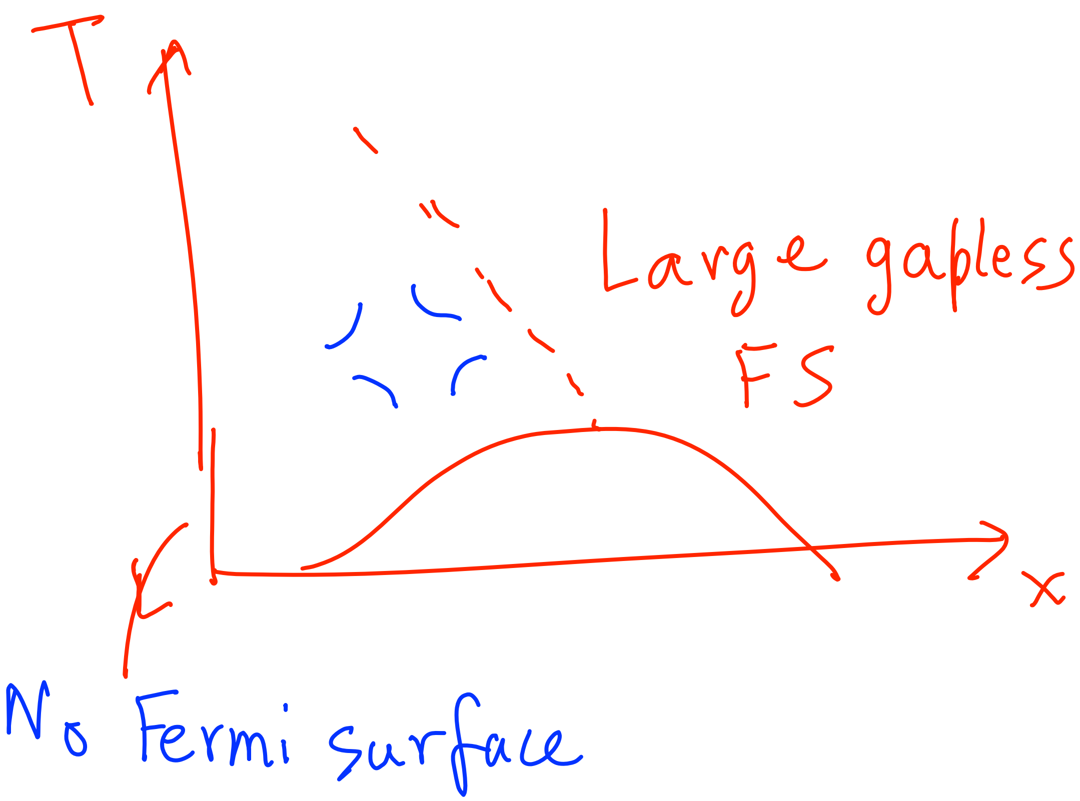
Mott insulator:
No Fermi surface

In SC state, the d-wave gap is centered on the large Fermi surface down to low doping.

A basic question

Quite generally, large Fermi surface visible (at least at short time scales) already in underdoped.

How should we understand the emergence of the large Fermi surface in a doped Mott insulator?



Theory: How does the Fermi surface die?

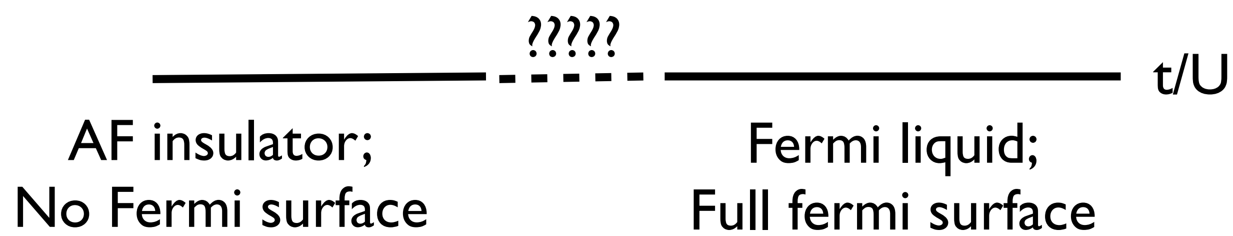
Motivates general study of how metal emerges from a Mott insulator.

The electronic Mott transition

Difficult old problem in quantum many body physics

How does a metal evolve into a Mott insulator?

Prototype: One band Hubbard model at half-filling on non-bipartite lattice



Why hard?

1. No order parameter for the metal-insulator transition

2. Need to deal with gapless Fermi surface on metallic side

3. Complicated interplay between metal-insulator transition and magnetic phase transition

Typically in most materials the Mott transition is first order.

But (at least on frustrated lattices) transition is sometimes only weakly first order
- fluctuation effects visible in approach to Mott insulator from metal.

Quantum spin liquid Mott insulators:

Opportunity for progress on the Mott transition -
- study metal-insulator transition without complications of magnetism.

Some candidate spin liquid materials

$\kappa - (ET)_2Cu_2(CN)_3$

$EtMe_3Sb[Pd(dmit)_2]_2$

Quasi-2d, approximately isotropic triangular lattice; best studied candidate spin liquids

$Na_4Ir_3O_8$

Three dimensional `hyperkagome' lattice

$ZnCu_3(OH)_6Cl_2$

Volborthtite, ...

2d Kagome lattice (`strong' Mott insulator)

Some candidate materials

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Quasi-2d, approximately isotropic triangular lattice; best studied candidate spin liquids

$Na_4Ir_3O_8$

Three dimensional `hyperkagome' lattice

Close to pressure driven Mott transition: `weak' Mott insulators

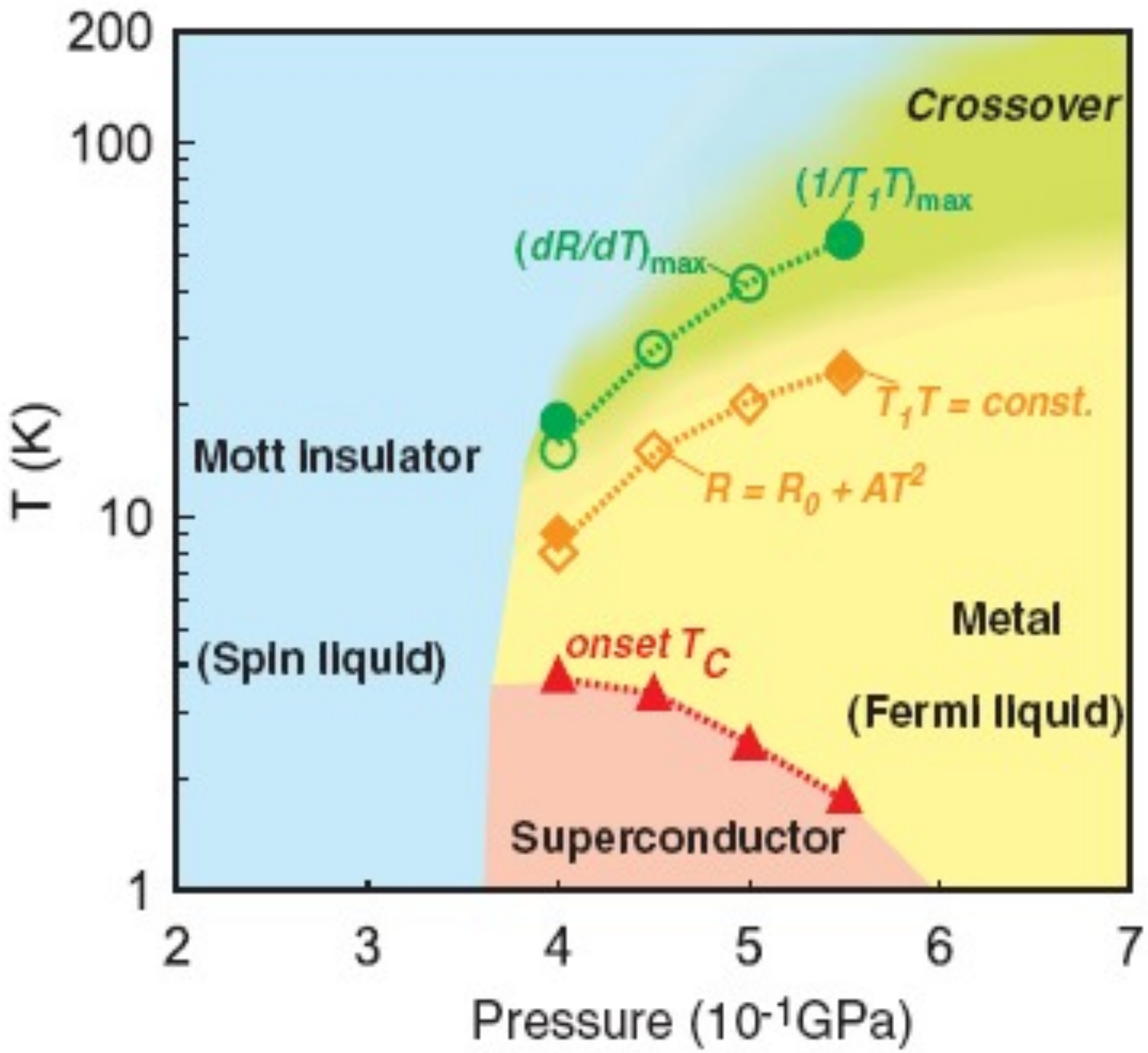
$ZnCu_3(OH)_6Cl_2$

Volborthtite, ...

2d Kagome lattice (`strong' Mott insulator)

Possible experimental realization of a second order(?) Mott transition

Kanoda et al '03 - '08



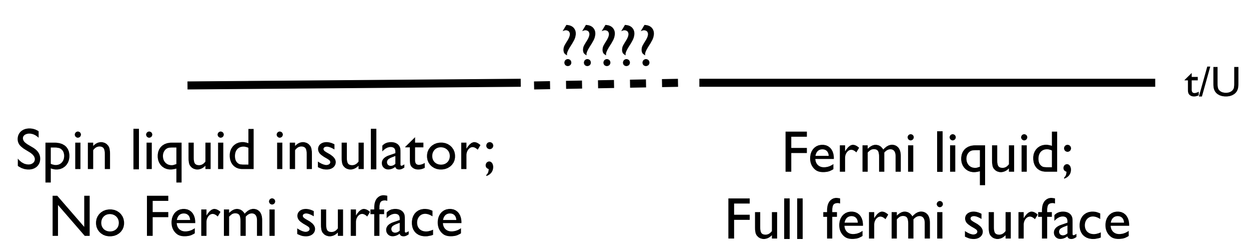
$\kappa-(ET)_2Cu_2(CN)_3$
under pressure

Quantum spin liquids and the Mott transition

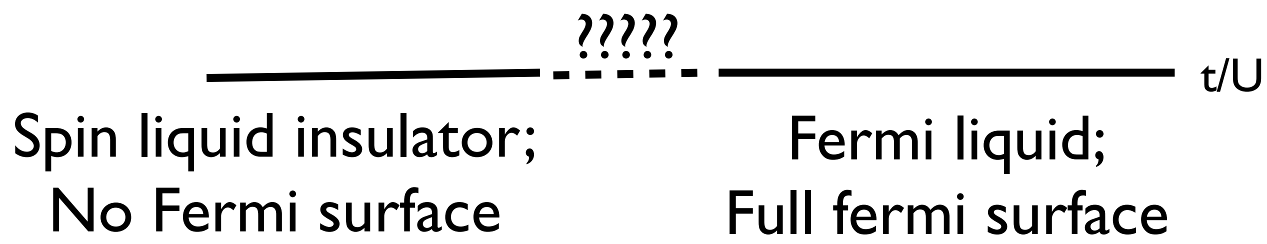
Some questions:

1. Can the Mott transition be continuous?

2. Fate of the electronic Fermi surface?



Killing the Fermi surface



At half-filling, through out metallic phase,
Luttinger theorem => size of Fermi surface is fixed.

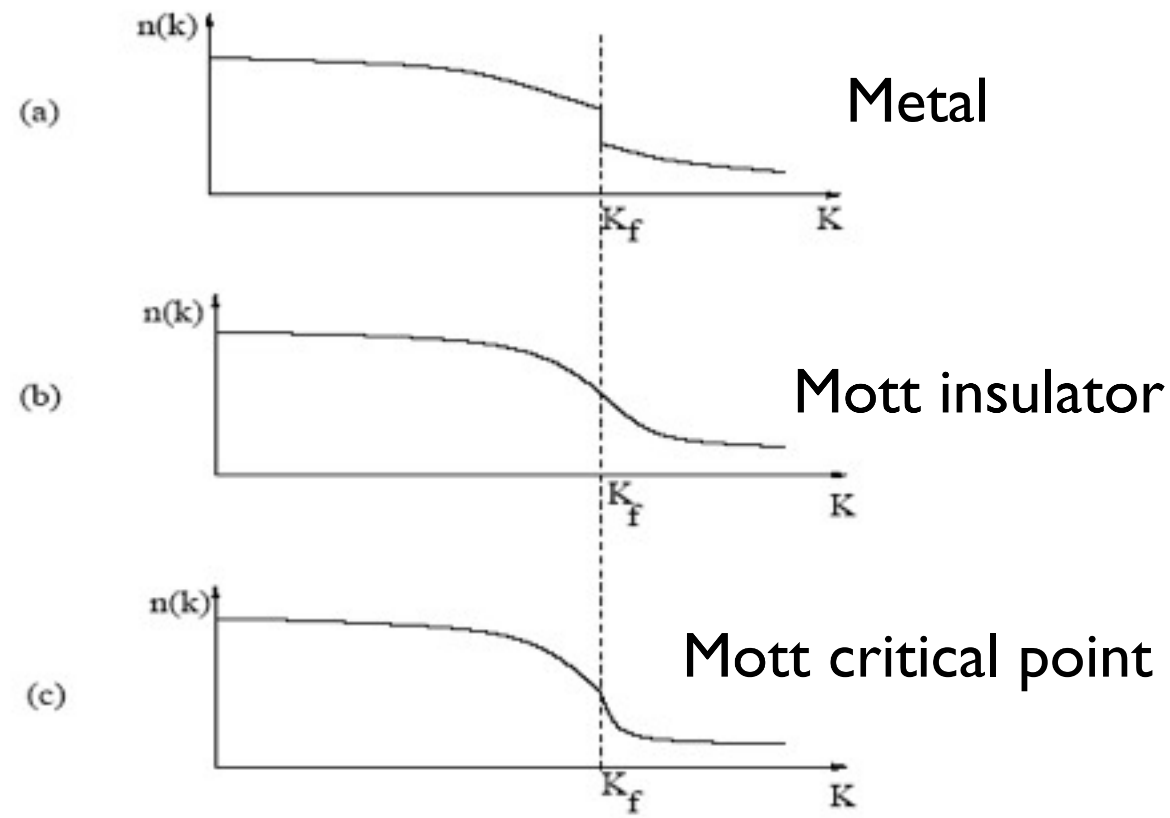
Approach to Mott insulator: entire Fermi surface must
die while maintaining size (cannot shrink to zero).

If Mott transition is second order, critical point necessarily very unusual.

``Fermi surface on brink of disappearing" - expect non-Fermi liquid physics.

Similar ``killing of Fermi surface" also at Kondo breakdown transition
in heavy fermion metals, and may be also around optimal doping in cuprates.

How can a Fermi surface die continuously?



Continuous disappearance of Fermi surface if quasiparticle weight Z vanishes continuously everywhere on the Fermi surface (Brinkman, Rice, 1970).

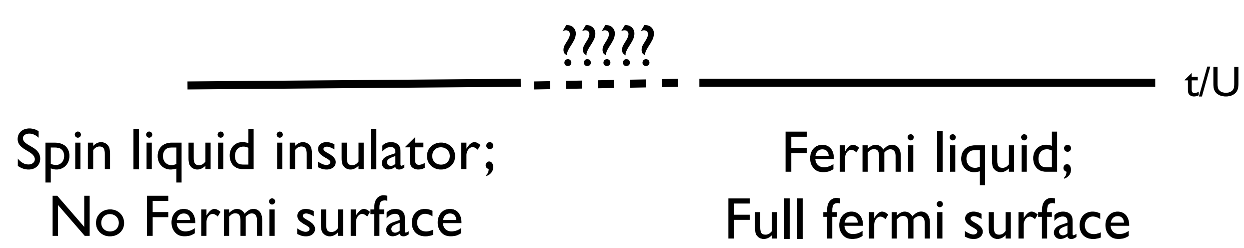
Concrete examples: DMFT in infinite d (Vollhardt, Metzner, Kotliar, Georges 1990s), slave particle theories in d = 2, d = 3 (TS, Vojta, Sachdev 2003, TS 2008)

Quantum spin liquids and the Mott transition

Some questions:

1. Can the Mott transition be continuous at T = 0?

2. Fate of the electronic Fermi surface?



Only currently available theoretical framework to answer these questions is slave particle gauge theory.

(Mean field: Florens, Georges 2005;
Spin liquid phase: Motrunich, 07, S.S. Lee, P.A. Lee, 07)

Slave particle framework

Split electron operator

$$c_{r\sigma} = b_r f_{r\alpha}$$

Fermi liquid: $\langle b \rangle \neq 0$

Mott insulator: b_r gapped

Mott transition: b_r critical

In all three cases $f_{r\alpha}$ form a Fermi surface.

Low energy effective theory: Couple b, f to fluctuating $U(1)$ gauge field.

Example: lattice Hubbard model

$$H = -\sum_{ij}\sum_{\alpha} t_{ij}\left(c^{\dagger}_{i\alpha}c_{j\alpha} + h.c\right) + U\sum_{i}\frac{n_i\left(n_i - 1\right)}{2} \tag{1}$$

Slave boson representation $c_{i\alpha} = b_i f_{i\alpha}$.

Factorize electron hopping as

$$\langle b_i^{\dagger} b_j\rangle f^{\dagger}_{i\alpha} f_{j\alpha} + b_i^{\dagger} b_j \langle f^{\dagger}_{i\alpha} f_{j\alpha}\rangle \tag{2}$$

Boson carries electron charge

=> Interaction term becomes a boson-boson interaction

`Mean field' description

Slave boson mean field theory:

$$H_{mf} = H_b + H_f \tag{1}$$

$$H_b = -t_c \sum_{<ij>} \left(b_i^\dagger b_j \right) + U \sum_i \frac{n_i(n_i - 1)}{2} \tag{2}$$

$$H_f = -\sum_{<ij>} t_{ij}^s \left(f_i^\dagger f_j + h.c \right) \tag{3}$$

Correlated metal: $t_c \gg U$, $< b > \neq 0$.

Mott insulator: $U \gg t_c$, bosons from a Mott insulator while fermions form a Fermi surface (i.e, a quantum spin liquid with spinon Fermi surface).

Readily generalize to other distinct quantum spin liquid states (eg BCS pairing of spinons).

Description of correlated metal

$$b \text{ condensed}, <b> \neq 0$$
$$=> c_{r\sigma} =< b > f_{r\sigma}$$
$$\text{Electron Green's function } < c\bar{c} > \approx | < b > |^2 < f\bar{f}\rangle$$
$$=> \text{Quasiparticle residue } Z = | < b > |^2$$

Quantum spin liquids and the Mott transition

1. Can the Mott transition be continuous?

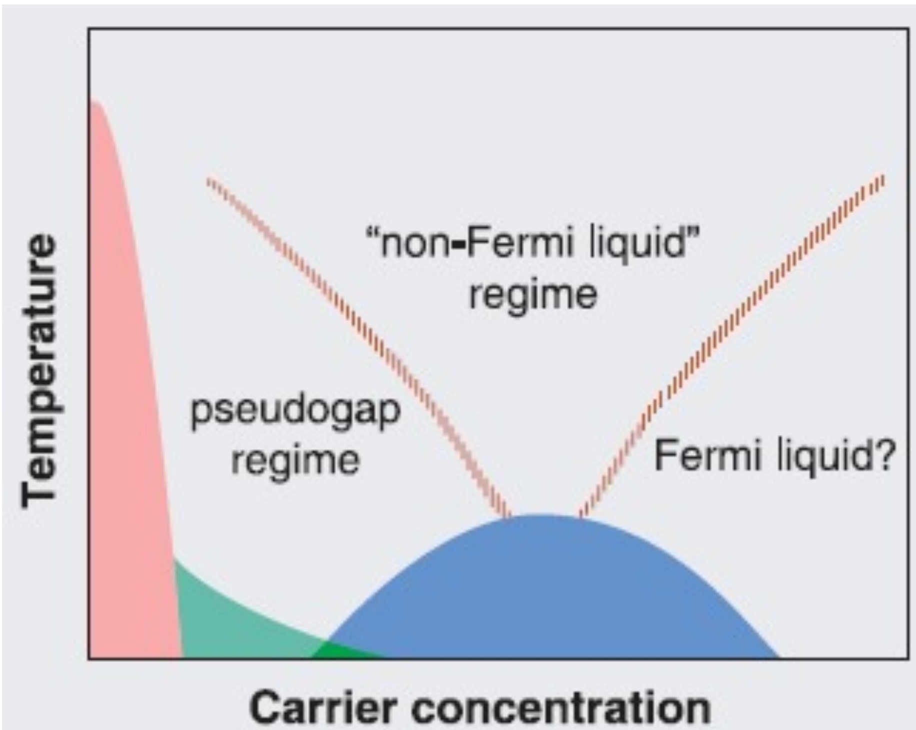
2. Fate of the electronic Fermi surface?

Analyse fluctuations: Concrete tractable theory of a continuous Mott transition; demonstrate critical Fermi surface at Mott transition;

Definite predictions for many quantities (TS, 2008, Witczak-Krempa, Ghaemi, Kim, TS, 2012).

- Universal jump of residual resistivity on approaching from metal
- Log divergent effective mass
- Two diverging time/length scales near transition
- Emergence of marginal fermi liquids

Superconductivity near a Mott transition



Some basic questions

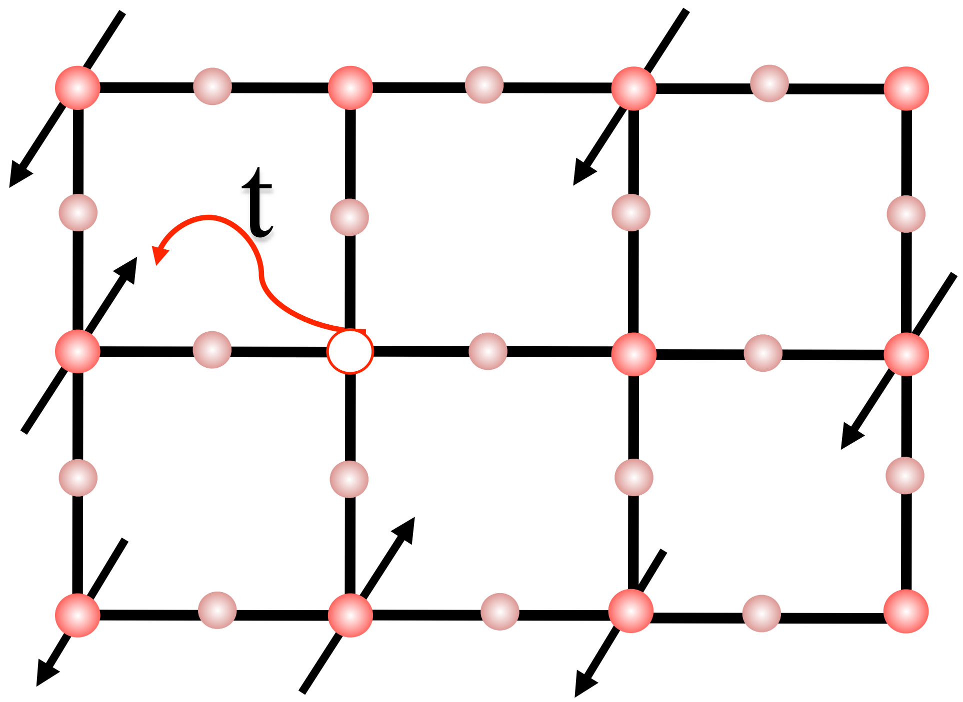
1.How does a
metal emerge from a Mott insulator?

2. Why superconductivity?

Simple physical picture (Anderson1987):
Superexchange favors formation of singlet valence bonds between localized spins.

Doped Mott insulator: Hole motion in background of valence bonds.

Cartoon pictures

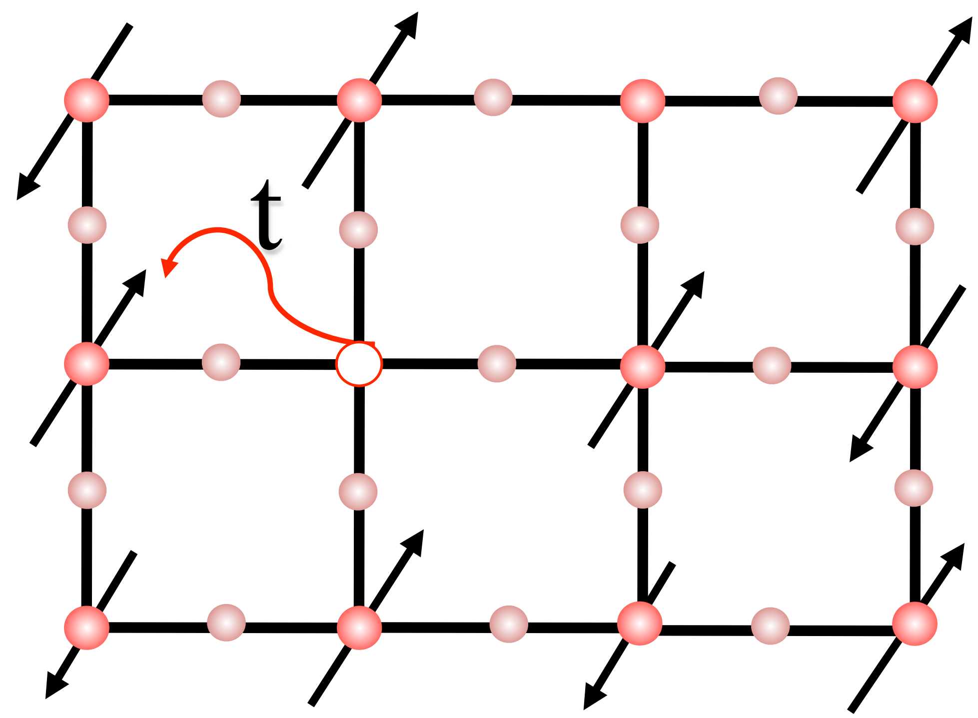


Large doping: Hubbard-U not very effective in blocking charge motion

Expect `large Fermi surface' with area set by 1-x.

What happens as doping is reduced to approach Mott insulator?

Cartoon pictures



Low doping: Most of the time most electrons unable to hop to neighboring sites due to Mott-blocking.

If electrons stay localized next to each other long enough, will develop superexchange which will lock their spins into singlets.

Electron configuration changes at long times – conveniently view as motion of holes in sea of singlets.

Resulting state: metallic but with a spin gap due to valence bond formation => `pseudogap metal".

Why superconductivity?

Crucial Anderson insight:

Singlet valence bond between localized spins: A localized Cooper pair.

\`Pairing' comes from superexchange due to a repulsive Hubbard interaction.

If spins were truly localized, Cooper pairs do not move => no superconductivity.

Nonzero doping: allow room for motion of valence bonds => superconductivity!

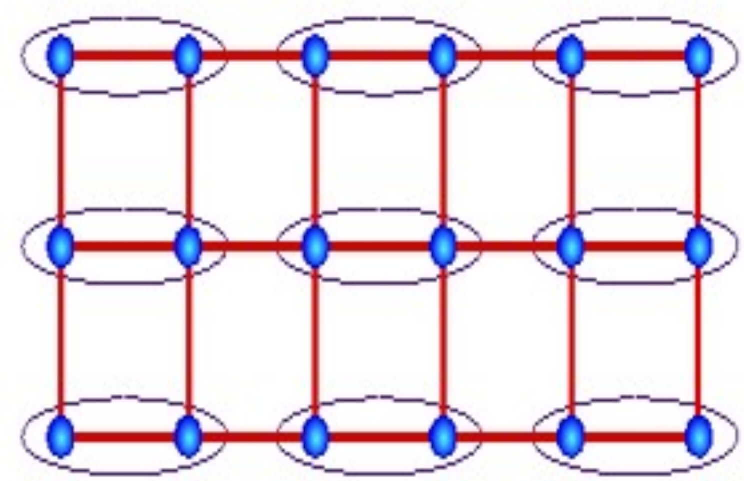
Hole picture: Coherent hole motion in valence bond sea

Fate of collection of valence bonds

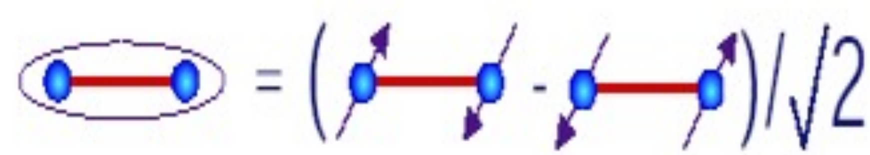
Two general possibilities:
Valence bonds can crystallize to form a solid (``Valence Bond Solid”)

OR

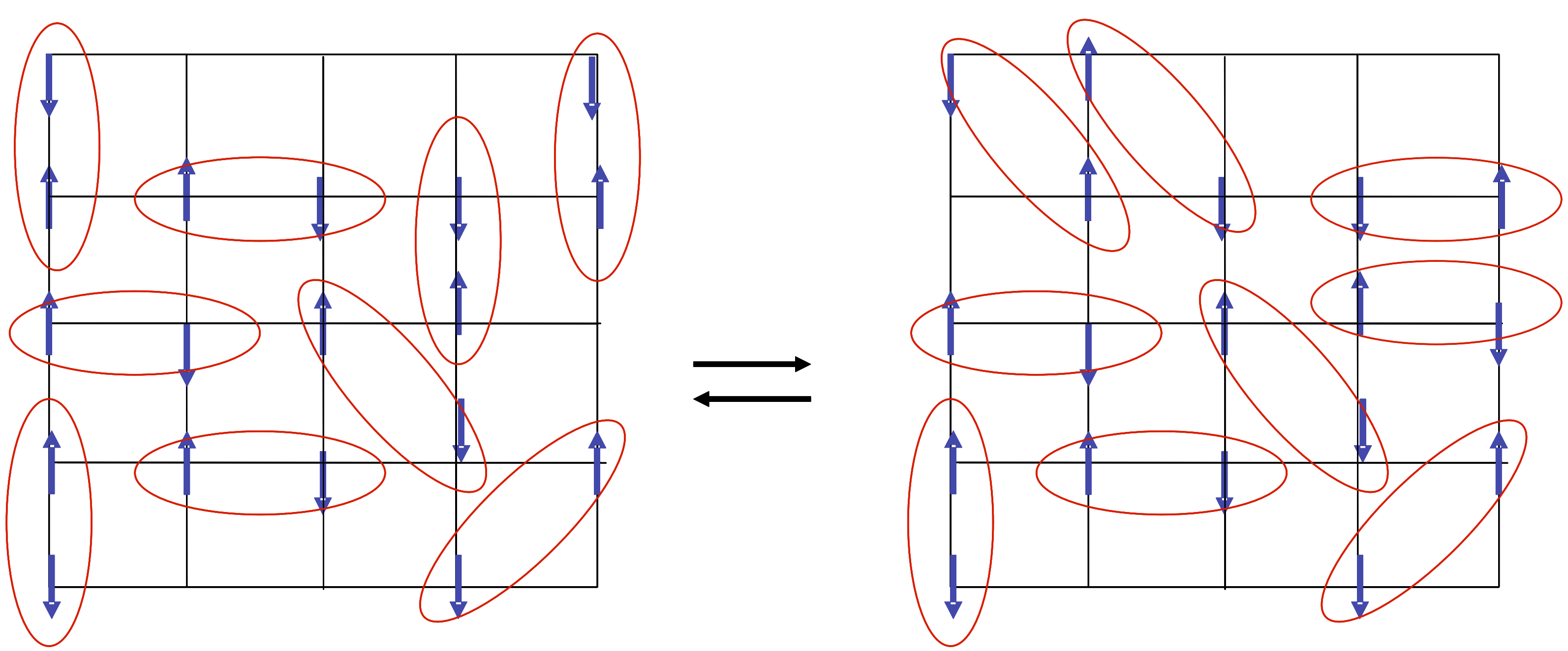
Stay liquid to form a `Resonating Valence Bond’



VBS state (with doping a `bond centered’ stripe)



Ongoing debates on which one is more relevant but very formation of valence bond crucial ingredient in much thinking about cuprates.

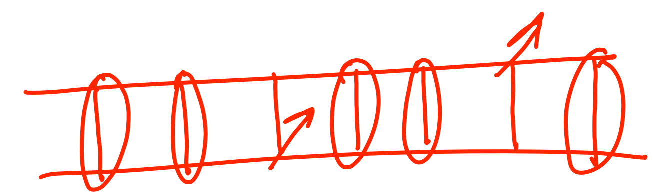


RVB state = quantum spin liquid

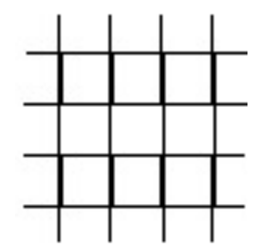
Does valence bond formation provide a legitimate <u>theoretical</u> route for superconductivity in a repulsive doped Mott insulator?

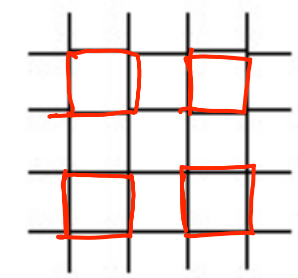
See Kivelson lectures

Many different kinds of studies (work of large number of people):



1.1d doped spin ladder:
Zero doping – spin gapped insulator due to valence bond formation.
Dope – (power law) superconductor .





2. Quasi-1d: Weakly coupled ladders

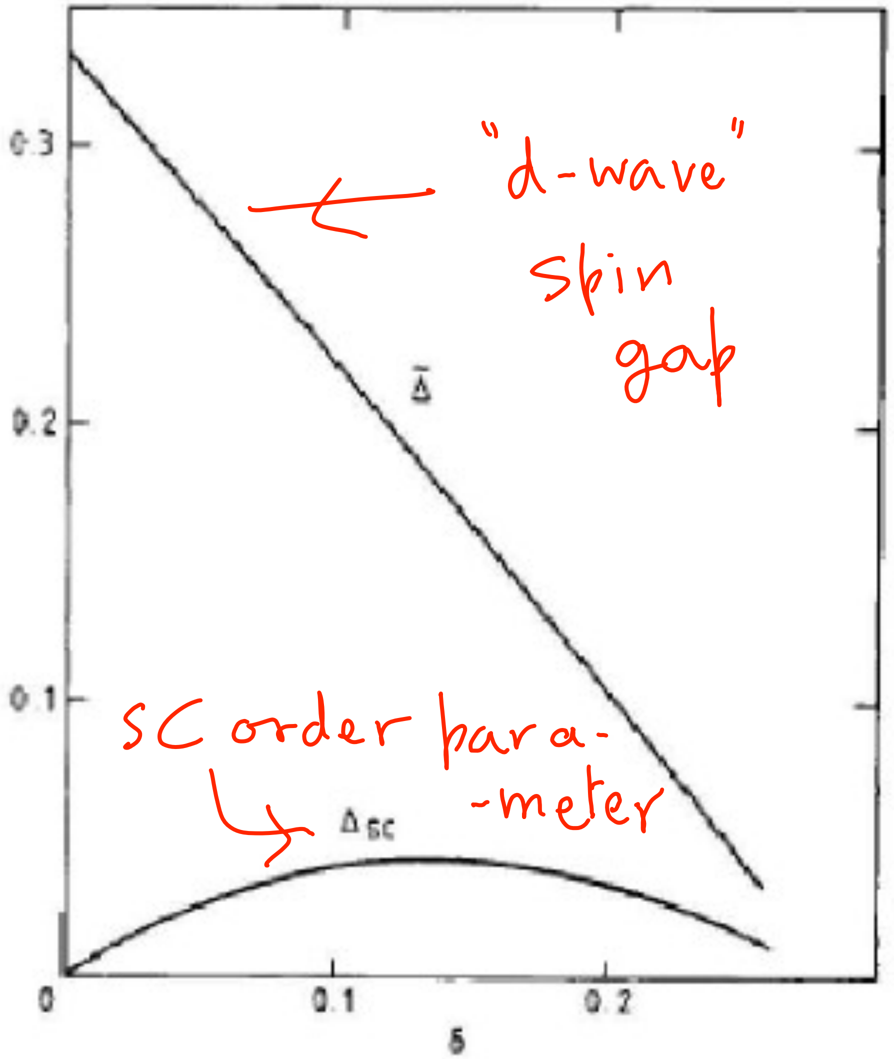
3. Inhomogenous 2d: Checkerboard Hubbard model

4. Superconductivity in doped VBS Mott insulators (`large-N' methods): spontaneously generate weakly coupled ladders.

5. Superconductivity in doped spin liquid Mott insulators (i.e insulators with one electron per site)

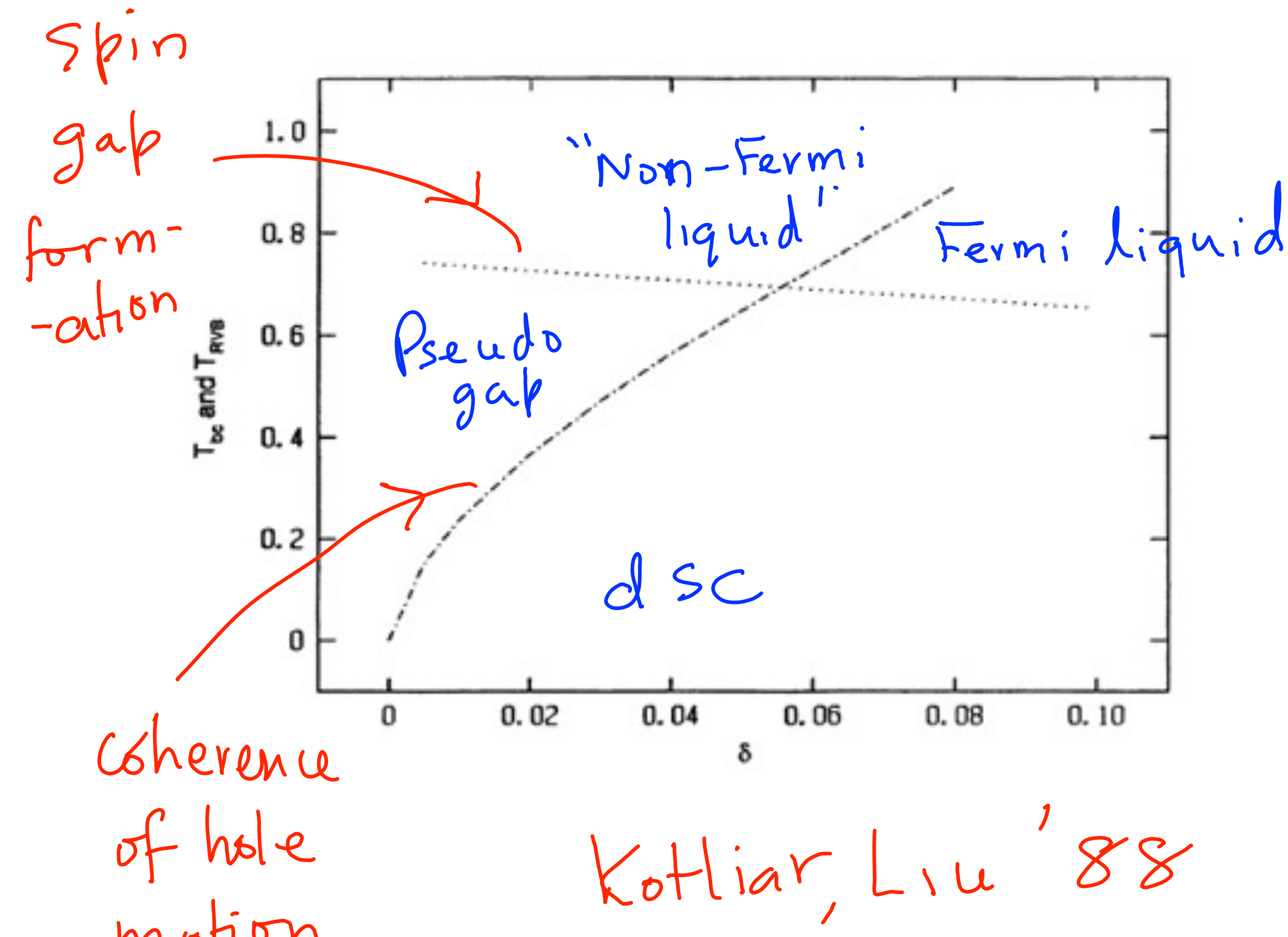
Superconductivity in doped spin liquids: mean field

Incorporate no double occupancy constraint of t-J model in approximate "mean field"



F.C. Zhang, Gros, Rice, Shiba '88

"Gutzwiller" mean field

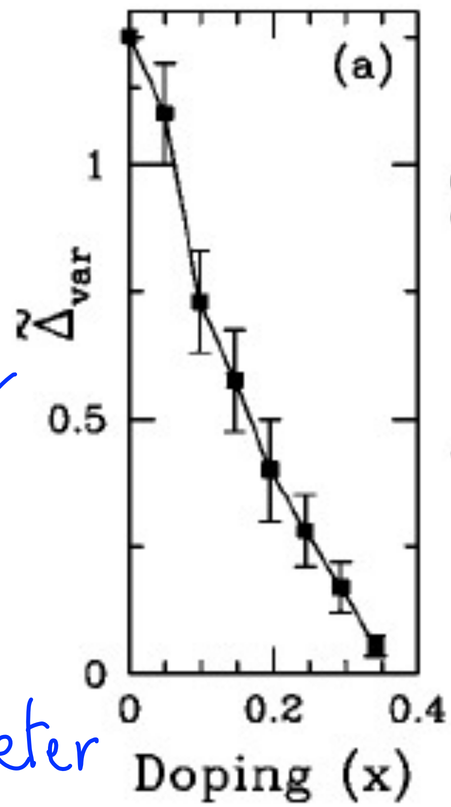


Kotliar, Liu '88

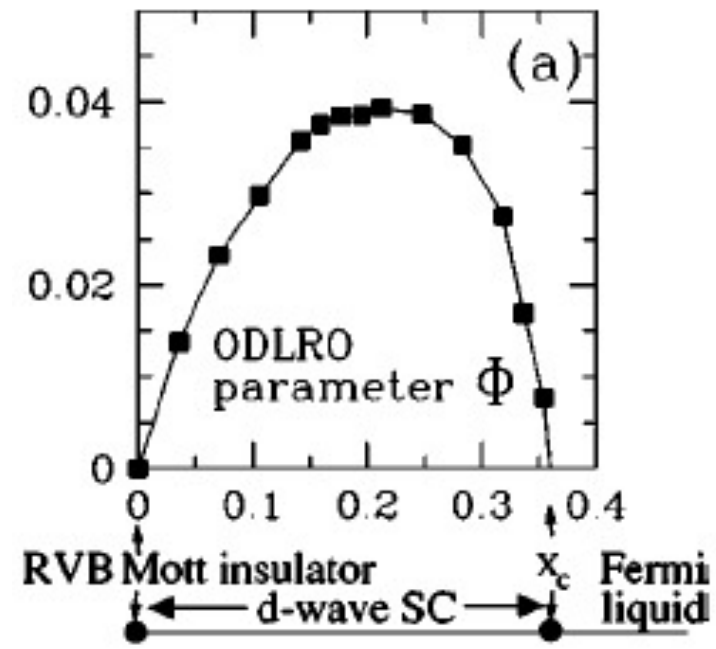
"Slave boson" mean field

Superconductivity in doped spin liquids: variational wavefunctions

$$|\Psi_{gd}\rangle = P_{\text{no double occupancy}} |dBCS\rangle$$



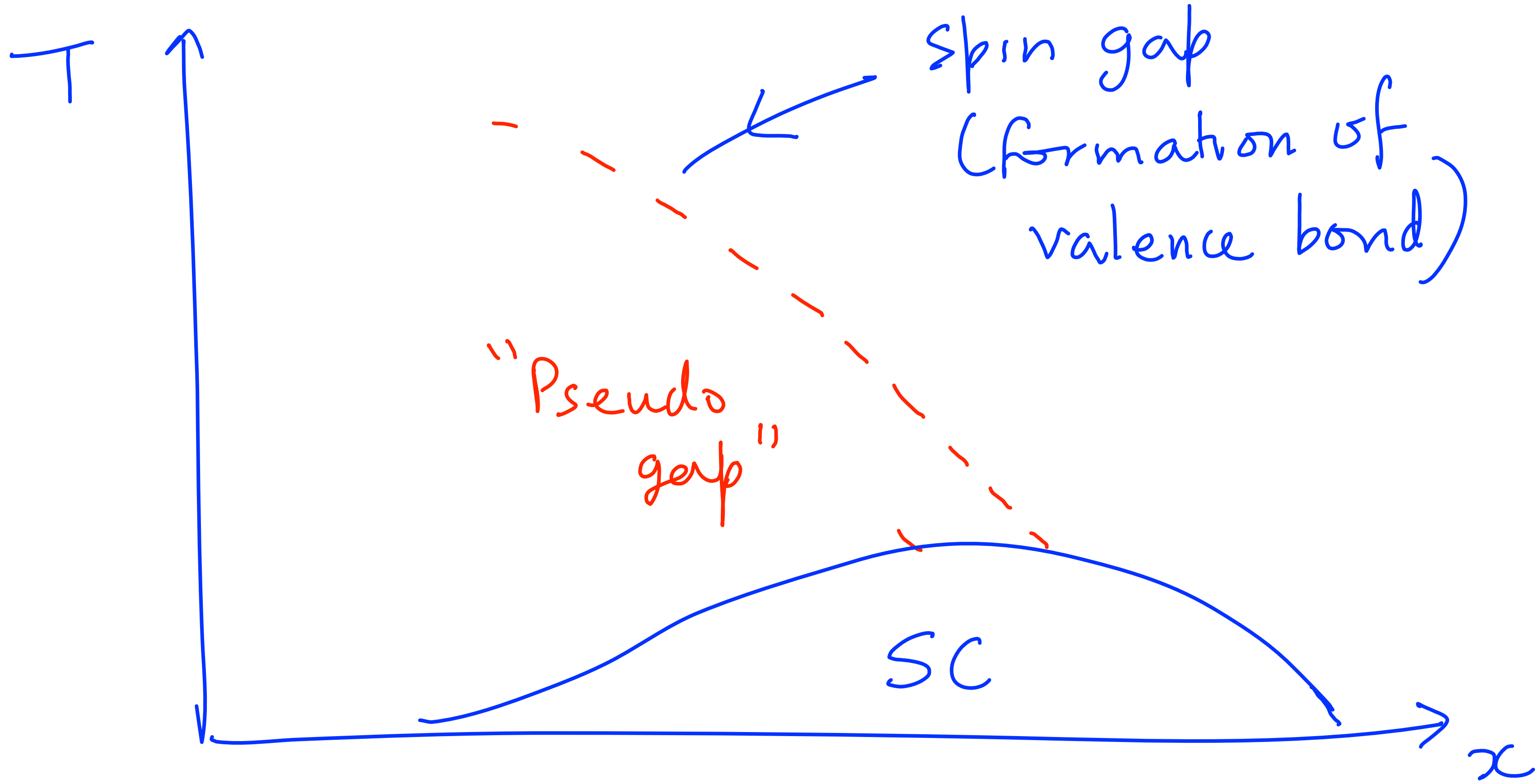
Gap parameter of $|dBCS\rangle$ in variational wave function



Paramekanti, Randeria, Trivedi 2001

Common features of superconductivity in doped (paramagnetic) Mott insulators

Generic phase diagram



"Low" x : T_c controlled by phase stiffness ρ_s ($\to 0$ as $x \to 0$)

Spins start gapping at higher temperature T^*

"High" x : T_c controlled by pairing gap $\searrow 0$

Refined basic theory questions

Is superconductivity with gapless nodal excitations possible in a doped Mott insulator?

Only currently known route is by doping a gapless spin liquid Mott insulator.

Eg: Z_2 spin liquid with d-wave pairing of fermionic spinons $\rightarrow$ d-wave SC with nodal quasiparticles.

Many similarities to physics of cuprates (more detail: Paremakanti lectures).

Comments

Quantum spin liquids a useful platform to understand the emergence of metals and superconductors from a Mott insulator.

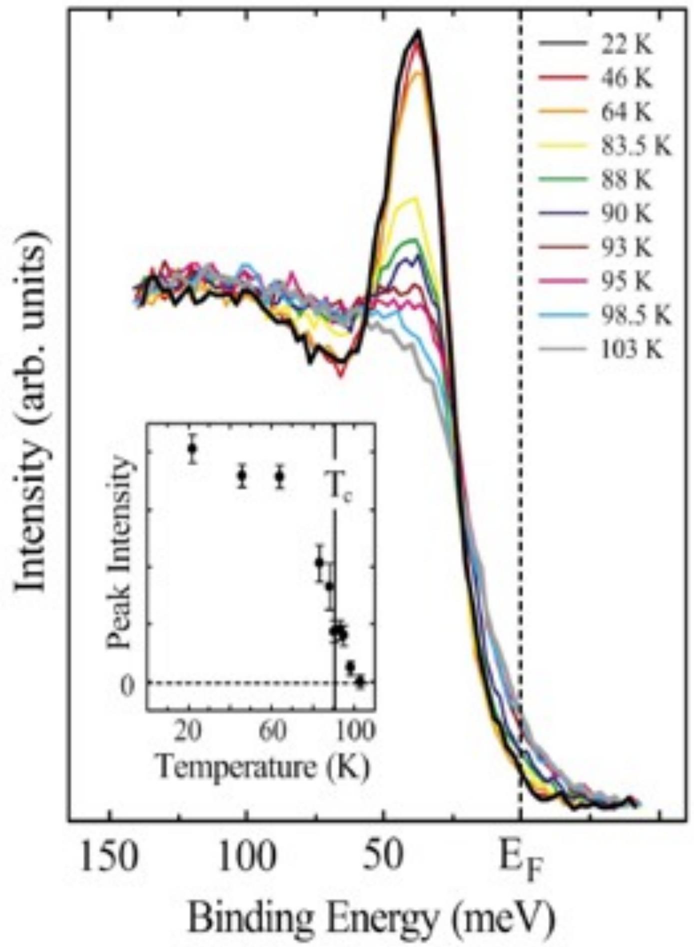
``Recognizable caricature” (to borrow from Sidney Coleman) of cuprate (and organics) physics

Direct relevance to cuprates?

Transition to SC: onset of coherence

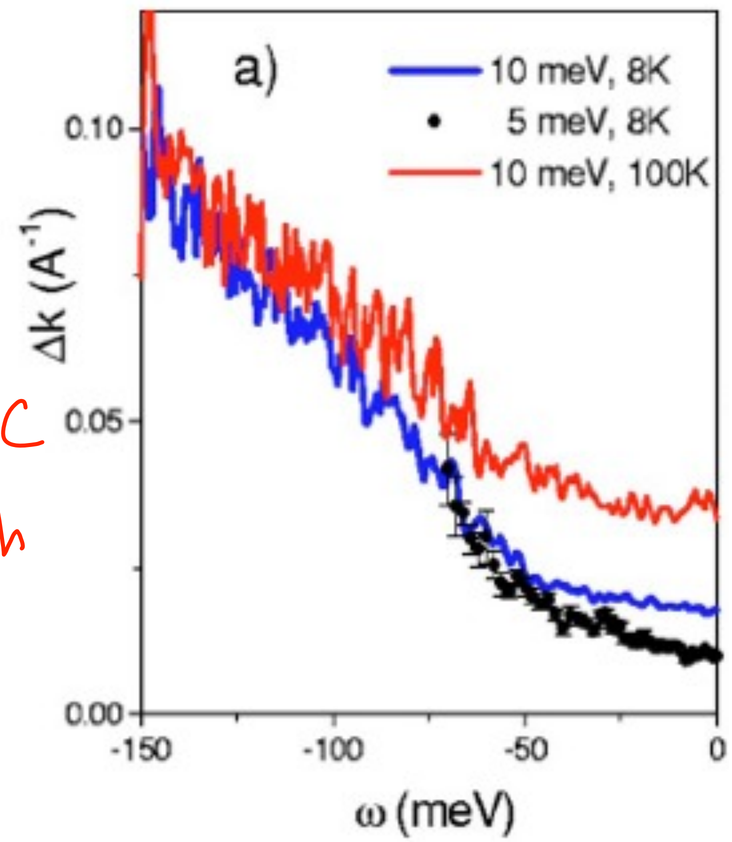
ARPES results

Anti node



Node

MDC width

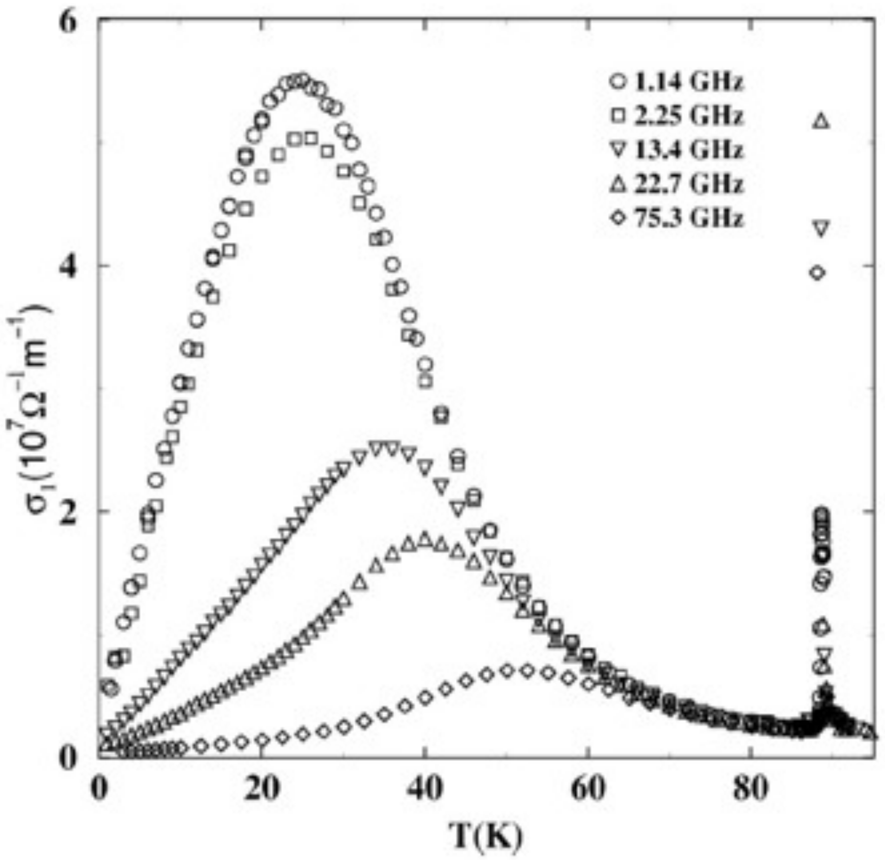


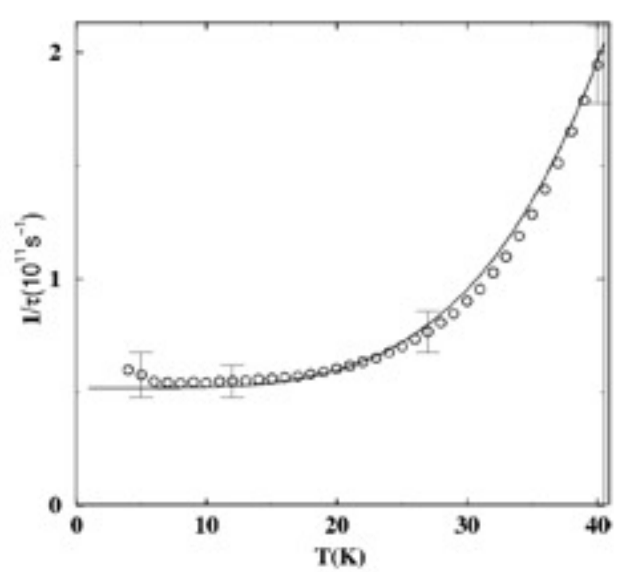
Sharp quasiparticles emerge for $T < T_c$.

Onset of coherence in transport

Microwave

Bonn, Hardy, et. al. '93, '99

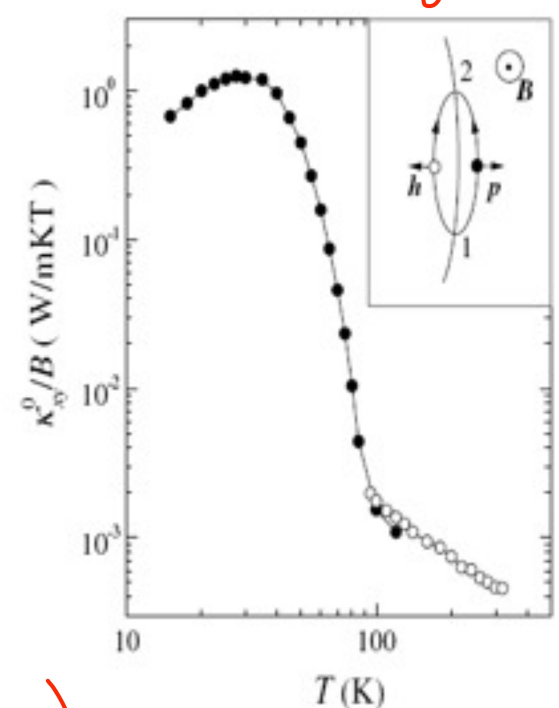


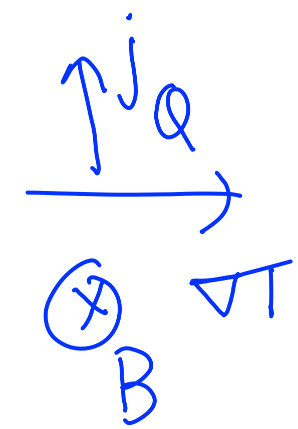


Thermal Hall effect

(Separate electron transport from phonon)

N. P. Ong '99





Collapse of scattering rate of nodal excitations for $T < T_c$.

Mean free paths ~ 1 micron